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TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	APR 04	STN AnaVist, Version 1, to be discontinued
NEWS	3	APR 15	WPIDS, WPINDEX, and WPIX enhanced with new predefined hit display formats
NEWS	4	APR 28	EMBASE Controlled Term thesaurus enhanced
NEWS	5	APR 28	IMSRESEARCH reloaded with enhancements
NEWS	6	MAY 30	INPAFAMDB now available on STN for patent family searching
NEWS	7	MAY 30	DGENE, PCTGEN, and USGENE enhanced with new homology sequence search option
NEWS	8	JUN 06	EPFULL enhanced with 260,000 English abstracts
NEWS	9	JUN 06	KOREAPAT updated with 41,000 documents
NEWS	10	JUN 13	USPATFULL and USPAT2 updated with 11-character patent numbers for U.S. applications
NEWS	11	JUN 19	CAS REGISTRY includes selected substances from web-based collections
NEWS	12	JUN 25	CA/CAPplus and USPAT databases updated with IPC reclassification data
NEWS	13	JUN 30	AEROSPACE enhanced with more than 1 million U.S. patent records
NEWS	14	JUN 30	EMBASE, EMBAL, and LEMBASE updated with additional options to display authors and affiliated organizations
NEWS	15	JUN 30	STN on the Web enhanced with new STN AnaVist Assistant and BLAST plug-in
NEWS	16	JUN 30	STN AnaVist enhanced with database content from EPFULL
NEWS	17	JUL 28	CA/CAPplus patent coverage enhanced
NEWS	18	JUL 28	EPFULL enhanced with additional legal status information from the epoline Register
NEWS	19	JUL 28	IFICDB, IFIPAT, and IFIUDB reloaded with enhancements
NEWS	20	JUL 28	STN Viewer performance improved
NEWS	21	AUG 01	INPADOCDB and INPAFAMDB coverage enhanced
NEWS	22	AUG 13	CA/CAPplus enhanced with printed Chemical Abstracts page images from 1967-1998
NEWS	23	AUG 15	CAOLD to be discontinued on December 31, 2008
NEWS	24	AUG 15	CAPplus currency for Korean patents enhanced
NEWS	25	AUG 25	CA/CAPplus, CASREACT, and IFI and USPAT databases enhanced for more flexible patent number searching
NEWS	26	AUG 27	CAS definition of basic patents expanded to ensure comprehensive access to substance and sequence information

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 08:22:26 ON 02 SEP 2008

=> FIL CAPLUS

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.84	0.84

FILE 'CAPLUS' ENTERED AT 08:24:39 ON 02 SEP 2008

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FILE COVERS 1907 - 2 Sep 2008 VOL 149 ISS 10
FILE LAST UPDATED: 1 Sep 2008 (20080901/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/legal/infopolicy.html>

=> D SAV

NAME	CREATED	NOTES/TITLE
ALL11134628/A	16 AUG 2007	2745 ANSWERS IN FILE CAPLUS

KAREN/A	13 JUL 2007	261 ANSWERS IN FILE CAPLUS
SER10534919/A	08 MAY 2008	761 ANSWERS IN FILE CAPLUS
STRUCTURE3/A	10 OCT 2007	9741 ANSWERS IN FILE CAPLUS
TOTALHITS/A	09 OCT 2007	12338 ANSWERS IN FILE REGISTRY
WHOLESET/A	07 JUL 2007	561 ANSWERS IN FILE CAPLUS

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=> ACT SER10534919/A
L1          STR
L2  (      10295)SEA FILE=REGISTRY SSS FUL L1
L3          761 SEA FILE=CAPLUS L2
```

```
=> FIL REG
COST IN U.S. DOLLARS          SINCE FILE      TOTAL
                               ENTRY      SESSION
FULL ESTIMATED COST          4.80          5.64
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FILE 'REGISTRY' ENTERED AT 08:30:46 ON 02 SEP 2008
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STRUCTURE FILE UPDATES: 1 SEP 2008 HIGHEST RN 1045602-82-1
DICTIONARY FILE UPDATES: 1 SEP 2008 HIGHEST RN 1045602-82-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

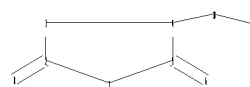
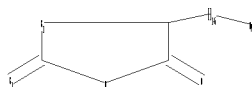
Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

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=> D SAVE
NAME          CREATED      NOTES/TITLE
-----
ALL11134628/A 16 AUG 2007  2745 ANSWERS IN FILE CAPLUS
KAREN/A        13 JUL 2007  261 ANSWERS IN FILE CAPLUS
SER10534919/A  08 MAY 2008  761 ANSWERS IN FILE CAPLUS
STRUCTURE3/A   10 OCT 2007  9741 ANSWERS IN FILE CAPLUS
TOTALHITS/A    09 OCT 2007  12338 ANSWERS IN FILE REGISTRY
WHOLESET/A     07 JUL 2007  561 ANSWERS IN FILE CAPLUS
```

```
=>
Uploading C:\Program Files\STNEXP\Queries\10534919\09_02_08_1.str
```



```

chain nodes :
6 8 10 11
ring nodes :
1 2 3 4 5
chain bonds :
2-8 4-10 5-6 10-11
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 2-8 3-4 4-5 4-10 5-6 10-11

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G1:C,O,S,N

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Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 8:Atom 10:CLASS 11:Atom
Generic attributes :
11:
Saturation          : Unsaturated

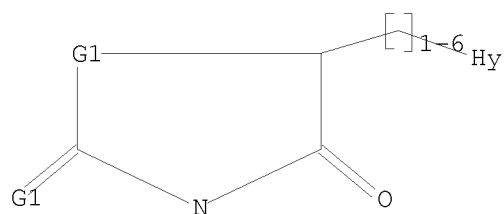
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L4 STRUCTURE UPLOADED

=> D

L4 HAS NO ANSWERS

L4 STR



G1 C,O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> S L4

SAMPLE SEARCH INITIATED 08:35:32 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 33663 TO ITERATE

5.9% PROCESSED 2000 ITERATIONS

23 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 662290 TO 684230

PROJECTED ANSWERS: 6562 TO 8922

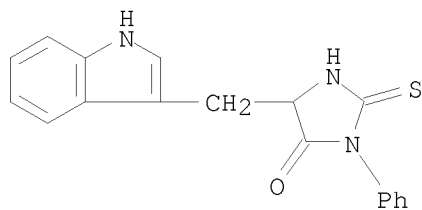
L5 23 SEA SSS SAM L4

=> D SCAN

L5 23 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN 4-Imidazolidinone, 5-(1H-indol-3-ylmethyl)-3-phenyl-2-thioxo-

MF C18 H15 N3 O S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> S L4 FUL

FULL SEARCH INITIATED 08:35:47 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 679408 TO ITERATE

100.0% PROCESSED 679408 ITERATIONS
SEARCH TIME: 00.00.09

6362 ANSWERS

L6 6362 SEA SSS FUL L4

=> FIL CAPLUS

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

182.04

187.68

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=> S L6

L7 1296 L6

=> FIL REG

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

1.44

189.12

FILE 'REGISTRY' ENTERED AT 08:37:53 ON 02 SEP 2008

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DICTIONARY FILE UPDATES: 1 SEP 2008 HIGHEST RN 1045602-82-1

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TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

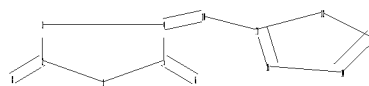
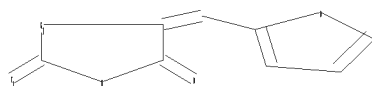
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

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Uploading C:\Program Files\STNEXP\Queries\10534919\09_02_08_2.str



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6 8 10

ring nodes :

1 2 3 4 5 11 12 13 14 15

chain bonds :

2-8 4-10 5-6 10-11

ring bonds :

1-2 1-5 2-3 3-4 4-5 11-12 11-15 12-13 13-14 14-15

exact/norm bonds :

1-2 1-5 2-3 2-8 3-4 4-5 4-10 5-6 10-11 11-12 11-15 12-13 13-14 14-15

G1:C,O,S,N

Match level :

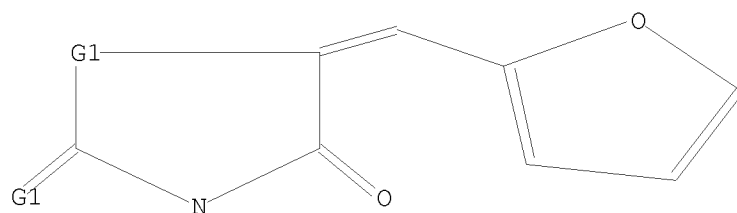
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13:Atom 14:Atom 15:Atom

L8 STRUCTURE UPLOADED

=> D

L8 HAS NO ANSWERS

L8 STR



G1 C,O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> S L8 FULL SUB=L6

FULL SUBSET SEARCH INITIATED 08:38:19 FILE 'REGISTRY'

FULL SUBSET SCREEN SEARCH COMPLETED - 208 TO ITERATE

100.0% PROCESSED 208 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L9 0 SEA SUB=L6 SSS FUL L8

=> S L8 FULL

FULL SEARCH INITIATED 08:38:43 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 36461 TO ITERATE

100.0% PROCESSED 36461 ITERATIONS

13753 ANSWERS

SEARCH TIME: 00.00.01

L10 13753 SEA SSS FUL L8

=> D HIS

(FILE 'HOME' ENTERED AT 08:22:26 ON 02 SEP 2008)

FILE 'CAPLUS' ENTERED AT 08:24:39 ON 02 SEP 2008

ACT SER10534919/A

L1 STR

L2 (10295)SEA FILE=REGISTRY SSS FUL L1

L3 761 SEA FILE=CAPLUS L2

FILE 'REGISTRY' ENTERED AT 08:30:46 ON 02 SEP 2008

L4 STRUCTURE UPLOADED

L5 23 S L4

L6 6362 S L4 FUL

FILE 'CAPLUS' ENTERED AT 08:36:19 ON 02 SEP 2008

L7 1296 S L6

FILE 'REGISTRY' ENTERED AT 08:37:53 ON 02 SEP 2008

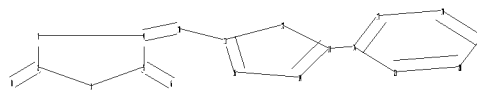
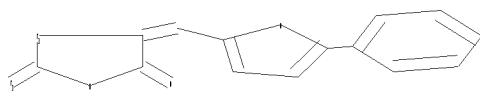
L8 STRUCTURE UPLOADED

L9 0 S L8 FULL SUB=L6

L10 13753 S L8 FULL

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Uploading C:\Program Files\STNEXP\Queries\10534919\09_02_08_3.str



chain nodes :

6 8 10

ring nodes :

1 2 3 4 5 11 12 13 14 15 16 17 18 19 20 21

chain bonds :

2-8 4-10 5-6 10-11 13-16

ring bonds :

1-2 1-5 2-3 3-4 4-5 11-12 11-15 12-13 13-14 14-15 16-17 16-21 17-18

18-19 19-20 20-21

exact/norm bonds :

1-2 1-5 2-3 2-8 3-4 4-5 4-10 5-6 10-11 11-12 11-15 12-13 13-14 13-16
14-15

normalized bonds :

16-17 16-21 17-18 18-19 19-20 20-21

G1:C,O,S,N

Match level :

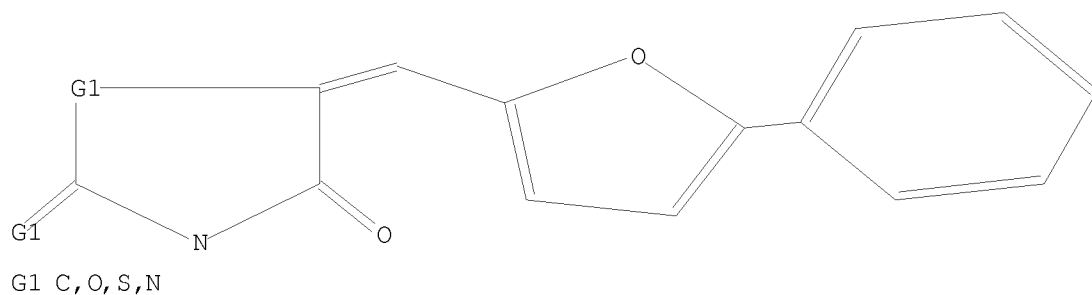
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13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom

L11 STRUCTURE UPLOADED

=> D

L11 HAS NO ANSWERS

L11 STR



Structure attributes must be viewed using STN Express query preparation.

=> S L11 FULL SUB=L10

FULL SUBSET SEARCH INITIATED 08:40:36 FILE 'REGISTRY'

FULL SUBSET SCREEN SEARCH COMPLETED - 9044 TO ITERATE

100.0% PROCESSED 9044 ITERATIONS

8915 ANSWERS

SEARCH TIME: 00.00.01

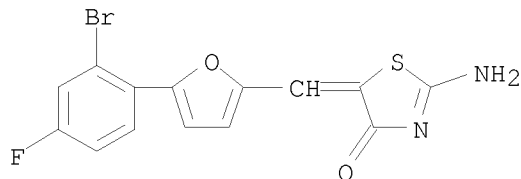
L12 8915 SEA SUB=L10 SSS FUL L11

=> D SCAN

L12 8915 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN 4(5H)-Thiazolone, 2-amino-5-[[5-(2-bromo-4-fluorophenyl)-2-furanyl]methylene]-

MF C14 H8 Br F N2 O2 S

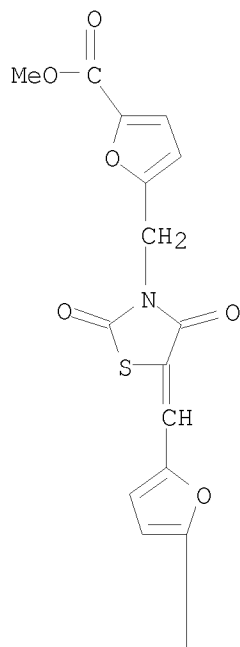


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

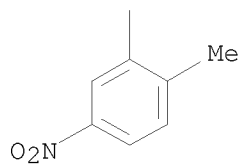
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L12 8915 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 2-Furancarboxylic acid, 5-[[5-[[5-(2-methyl-5-nitrophenyl)-2-
furanyl]methylene]-2,4-dioxo-3-thiazolidinyl]methyl]-, methyl ester
MF C22 H16 N2 O8 S

PAGE 1-A



PAGE 2-A



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> FIL CAPLUS

COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE

ENTRY

266.24

TOTAL

SESSION

455.36

FILE 'CAPLUS' ENTERED AT 08:43:11 ON 02 SEP 2008

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Searched by Jason M. Nolan, Ph.D.

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<http://www.cas.org/legal/infopolicy.html>

=> D HIS

(FILE 'HOME' ENTERED AT 08:22:26 ON 02 SEP 2008)

FILE 'CAPLUS' ENTERED AT 08:24:39 ON 02 SEP 2008
ACT SER10534919/A

L1 STR
L2 (10295)SEA FILE=REGISTRY SSS FUL L1
L3 761 SEA FILE=CAPLUS L2

FILE 'REGISTRY' ENTERED AT 08:30:46 ON 02 SEP 2008
L4 STRUCTURE UPLOADED
L5 23 S L4
L6 6362 S L4 FUL

FILE 'CAPLUS' ENTERED AT 08:36:19 ON 02 SEP 2008
L7 1296 S L6

FILE 'REGISTRY' ENTERED AT 08:37:53 ON 02 SEP 2008
L8 STRUCTURE UPLOADED
L9 0 S L8 FULL SUB=L6
L10 13753 S L8 FULL
L11 STRUCTURE UPLOADED
L12 8915 S L11 FULL SUB=L10

FILE 'CAPLUS' ENTERED AT 08:43:11 ON 02 SEP 2008

=> S L12

L13 115 L12

=> S L13 AND COMPOSITION

735831 COMPOSITION

L14 1 L13 AND COMPOSITION

=> D IBIB

L14 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:981372 CAPLUS

DOCUMENT NUMBER: 142:274062

TITLE: Pharmaceutical composition comprising
2-chloro-5-[5-(2-imino-4-oxo-thiazolidin-5-yl
idenemethyl)-furan-2-yl]-benzoic acid derivatives for
inhibition of protein tyrosine phosphatase 1b activity

INVENTOR(S): Cho, Jung Myeong; Hwang, Gwang Yeon; Jun, Yeong Ho;
Kim, Jin Hwan; Lee, Tae Gyu; Noh, Seong Gu

PATENT ASSIGNEE(S): Crystalgenomics, Inc., S. Korea

SOURCE: Repub. Korean Kongkae Taeho Kongbo, No pp. given
CODEN: KRXXA7

DOCUMENT TYPE: Patent

LANGUAGE: Korean

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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KR 2003095730	A	20031224	KR 2002-33284	20020614
PRIORITY APPLN. INFO.:			KR 2002-33284	20020614

=> D IBIB ABS HITSTR L14

L14 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:981372 CAPLUS

DOCUMENT NUMBER: 142:274062

TITLE: Pharmaceutical composition comprising
2-chloro-5-[5-(2-imino-4-oxo-thiazolidin-5-yl
idenemethyl)-furan-2-yl]-benzoic acid derivatives for
inhibition of protein tyrosine phosphatase 1b activity

INVENTOR(S): Cho, Jung Myeong; Hwang, Gwang Yeon; Jun, Yeong Ho;
Kim, Jin Hwan; Lee, Tae Gyu; Noh, Seong Gu

PATENT ASSIGNEE(S): Crystalgenomics, Inc., S. Korea

SOURCE: Repub. Korean Kongkae Taeho Kongbo, No pp. given
CODEN: KRXXA7

DOCUMENT TYPE: Patent

LANGUAGE: Korean

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
KR 2003095730	A	20031224	KR 2002-33284	20020614
PRIORITY APPLN. INFO.:			KR 2002-33284	20020614

AB Provided is a pharmaceutical composition comprising 2-chloro-5-[5-(2-imino-4-oxo-thiazolidin-5-yl idenemethyl)-furan-2-yl]-benzoic acid derivs. to inhibit the activity of protein tyrosine phosphatase 1B(PTP 1B). It effectively inhibits the activity of PTP 1B and is thus used for the prevention and treatment of obesity or diabetes. A pharmaceutical composition

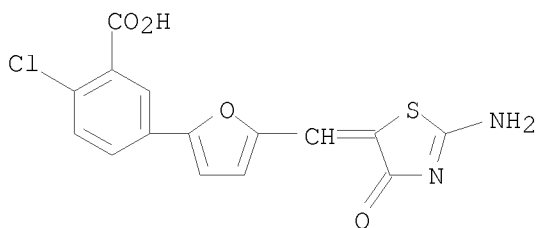
for the inhibit the activity of protein tyrosine phosphatase 1B(PTP 1B) is characterized by comprising 2-chloro-5-[5-(2-imino-4-oxo-thiazolidin-5-ylidenemethyl)-furan-2-yl]-benzoic acid derivs., their pharmaceutically acceptable salt, hydrate, solvate or isomer. In the formula, R1 is an aromatic group substituted or unsubstituted with at least one of halogen, alkyloxy, alkyl, amino, alkyl amino, carboxylic acid or amide; a nitrogen, sulfur or oxygen-containing aromatic group; or an aromatic group substituted or unsubstituted C1-C6 alkyl, and R2 is hydrogen; an aromatic group substituted or unsubstituted with at least one of halogen, alkyloxy, alkyl, amino, alkylamino, carboxylic acid or amide; a nitrogen, sulfur or oxygen-containing aromatic group; or an aromatic group substituted or unsubstituted C1-C6 alkyl, and R2 is hydrogen.

IT 401611-95-8 401611-95-8D, derivs.

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmaceutical composition comprising furan benzoic acid derivs. for inhibition of protein tyrosine phosphatase 1b activity)

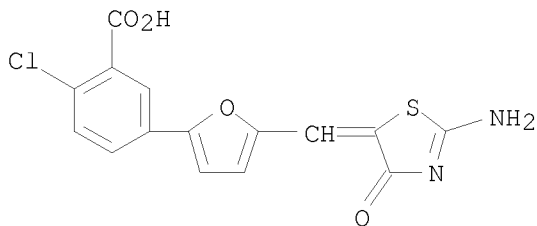
RN 401611-95-8 CAPLUS

CN Benzoic acid, 5-[5-[(2-amino-4-oxo-5(4H)-thiazolylidene)methyl]-2-furanyl]-2-chloro- (CA INDEX NAME)



RN 401611-95-8 CAPLUS

CN Benzoic acid, 5-[5-[(2-amino-4-oxo-5(4H)-thiazolylidene)methyl]-2-furanyl]-2-chloro- (CA INDEX NAME)



=> FIL REG

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

16.94

472.30

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-0.80

-0.80

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predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> D HIS

(FILE 'HOME' ENTERED AT 08:22:26 ON 02 SEP 2008)

FILE 'CAPLUS' ENTERED AT 08:24:39 ON 02 SEP 2008
ACT SER10534919/A

L1 STR
L2 (10295)SEA FILE=REGISTRY SSS FUL L1
L3 761 SEA FILE=CAPLUS L2

FILE 'REGISTRY' ENTERED AT 08:30:46 ON 02 SEP 2008
L4 STRUCTURE UPLOADED
L5 23 S L4
L6 6362 S L4 FUL

FILE 'CAPLUS' ENTERED AT 08:36:19 ON 02 SEP 2008
L7 1296 S L6

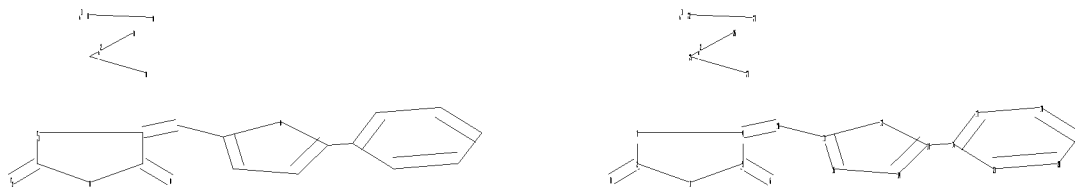
FILE 'REGISTRY' ENTERED AT 08:37:53 ON 02 SEP 2008
L8 STRUCTURE UPLOADED
L9 0 S L8 FULL SUB=L6
L10 13753 S L8 FULL
L11 STRUCTURE UPLOADED
L12 8915 S L11 FULL SUB=L10

FILE 'CAPLUS' ENTERED AT 08:43:11 ON 02 SEP 2008
L13 115 S L12
L14 1 S L13 AND COMPOSITION

FILE 'REGISTRY' ENTERED AT 08:53:37 ON 02 SEP 2008

=>

Uploading C:\Program Files\STNEXP\Queries\10534919\09_02_08_4.str



chain nodes :

6 8 10 22 23 25 26 27

ring nodes :

1 2 3 4 5 11 12 13 14 15 16 17 18 19 20 21

chain bonds :

2-8 4-10 5-6 10-11 13-16 22-23 25-26 25-27

ring bonds :

1-2 1-5 2-3 3-4 4-5 11-12 11-15 12-13 13-14 14-15 16-17 16-21 17-18
18-19 19-20 20-21

exact/norm bonds :

1-2 1-5 2-3 2-8 3-4 4-5 4-10 5-6 10-11 11-12 11-15 12-13 13-14 13-16
14-15 22-23 25-26 25-27

normalized bonds :

16-17 16-21 17-18 18-19 19-20 20-21

G1:C,O,S,N

G2:O,S,[*1],[*2]

Match level :

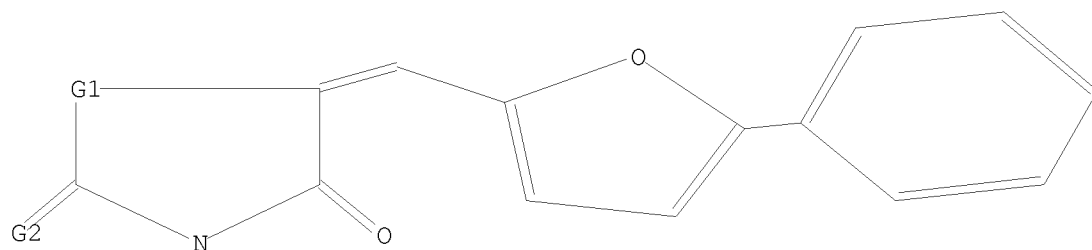
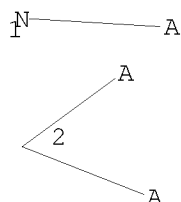
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 8:Atom 10:CLASS 11:Atom 12:Atom
13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:CLASS 23:CLASS 25:CLASS 26:CLASS 27:CLASS

L15 STRUCTURE UPLOADED

=> D

L15 HAS NO ANSWERS

L15 STR



G1 C,O,S,N

G2 O,S,[@1],[@2]

Structure attributes must be viewed using STN Express query preparation.

=> S L15 FULL SUB=L10

FULL SUBSET SEARCH INITIATED 08:54:30 FILE 'REGISTRY'

FULL SUBSET SCREEN SEARCH COMPLETED - 9040 TO ITERATE

100.0% PROCESSED 9040 ITERATIONS

6095 ANSWERS

SEARCH TIME: 00.00.01

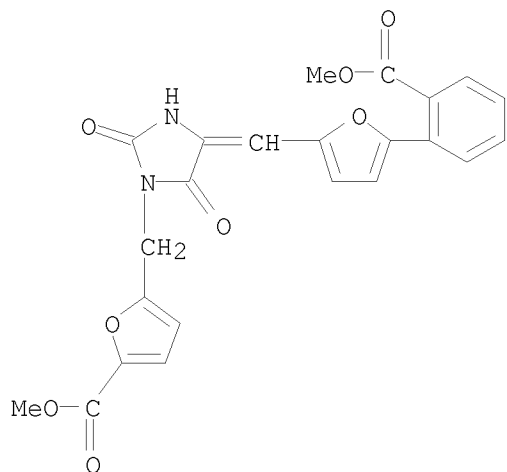
L16 6095 SEA SUB=L10 SSS FUL L15

=> D SCAN

L16 6095 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN 2-Furancarboxylic acid, 5-[[4-[[5-[2-(methoxycarbonyl)phenyl]-2-furanyl]methylene]-2,5-dioxo-1-imidazolidinyl]methyl]-, methyl ester

MF C23 H18 N2 O8



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> FIL CAPLUS

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

43.48

515.78

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

0.00

-0.80

FILE 'CAPLUS' ENTERED AT 08:55:17 ON 02 SEP 2008

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FILE COVERS 1907 - 2 Sep 2008 VOL 149 ISS 10

FILE LAST UPDATED: 1 Sep 2008 (20080901/ED)

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<http://www.cas.org/legal/infopolicy.html>

=> S L16

L17 107 L16

=> D IBIB ABS HISTSR 107

'HISTSR' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

The following are valid formats:

ABS ----- GI and AB
 ALL ----- BIB, AB, IND, RE
 APPS ----- AI, PRAI
 BIB ----- AN, plus Bibliographic Data and PI table (default)
 CAN ----- List of CA abstract numbers without answer numbers
 CBIB ----- AN, plus Compressed Bibliographic Data
 CLASS ----- IPC, NCL, ECLA, FTERM
 DALL ----- ALL, delimited (end of each field identified)
 DMAX ----- MAX, delimited for post-processing
 FAM ----- AN, PI and PRAI in table, plus Patent Family data
 FBIB ----- AN, BIB, plus Patent FAM
 IND ----- Indexing data
 IPC ----- International Patent Classifications
 MAX ----- ALL, plus Patent FAM, RE
 PATS ----- PI, SO
 SAM ----- CC, SX, TI, ST, IT
 SCAN ----- CC, SX, TI, ST, IT (random display, no answer numbers;
 SCAN must be entered on the same line as the DISPLAY,
 e.g., D SCAN or DISPLAY SCAN)
 STD ----- BIB, CLASS

 IABS ----- ABS, indented with text labels
 IALL ----- ALL, indented with text labels
 IBIB ----- BIB, indented with text labels
 IMAX ----- MAX, indented with text labels
 ISTD ----- STD, indented with text labels

 OBIB ----- AN, plus Bibliographic Data (original)
 OIBIB ----- OBIB, indented with text labels

 SBIB ----- BIB, no citations
 SIBIB ----- IBIB, no citations

 HIT ----- Fields containing hit terms
 HITIND ----- IC, ICA, ICI, NCL, CC and index field (ST and IT)
 containing hit terms
 HITRN ----- HIT RN and its text modification
 HITSTR ----- HIT RN, its text modification, its CA index name, and
 its structure diagram
 HITSEQ ----- HIT RN, its text modification, its CA index name, its
 structure diagram, plus NTE and SEQ fields
 FHITSTR ----- First HIT RN, its text modification, its CA index name, and
 its structure diagram
 FHITSEQ ----- First HIT RN, its text modification, its CA index name, its

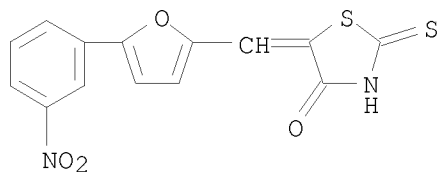
structure diagram, plus NTE and SEQ fields
KWIC ----- Hit term plus 20 words on either side
OCC ----- Number of occurrence of hit term and field in which it occurs

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of formats include: TI; TI,AU; BIB,ST; TI,IND; TI,SO. You may specify the format fields in any order and the information will be displayed in the same order as the format specification.

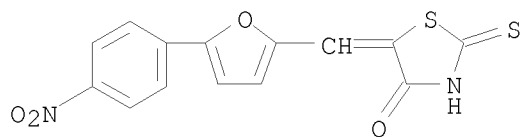
All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR, FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC to view a specified Accession Number.
ENTER DISPLAY FORMAT (BIB):END

=> D IBIB ABS HITSTR L17 107

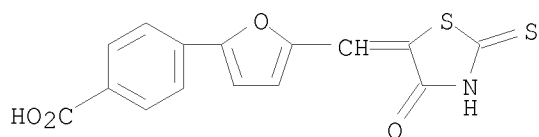
L17 ANSWER 107 OF 107 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1972:59507 CAPLUS
DOCUMENT NUMBER: 76:59507
ORIGINAL REFERENCE NO.: 76:9589a,9592a
TITLE: Furan derivatives XXIV. Synthesis of substituted
5-(5-phenyl-2-furfurylidene)rhodanines
AUTHOR(S): Krutosikova, A.; Frimm, R.; Kovac, J.
CORPORATE SOURCE: Inst. Org. Chem., Slovak Tech. Univ., Bratislava,
Czech.
SOURCE: Sbornik Prac Chemickej Fakulty SVST (1971), Volume
Date 1969-1970 55-8
CODEN: SCFSAL; ISSN: 0520-7339
DOCUMENT TYPE: Journal
LANGUAGE: Slovak
GI For diagram(s), see printed CA Issue.
AB With the object of preparing biol. active agents of low toxicity, title
comps. (I) were prepared by boiling a mixture of the appropriately
substituted 5-phenyl-2-furaldehyde, rhodanine, and AcONa in AcOH 30 min.
The following I were prepared (R and % yield given): 4-O2N, 81; 3-O2N, 87;
2-O2N, 92; 4-HO2C, 87; 4-Cl, 86; 4-Br, 77; 4-EtO2C, 80; H, 92; 4-Me, 49;
4-MeO, 51.
IT 35274-35-2P 35274-36-3P 35274-37-4P
35274-38-5P 35274-39-6P 35274-40-9P
35274-41-0P 35274-42-1P 35386-81-3P
36405-07-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35274-35-2 CAPLUS
CN 4-Thiazolidinone, 5-[[5-(3-nitrophenyl)-2-furanyl]methylene]-2-thioxo-
(CA INDEX NAME)



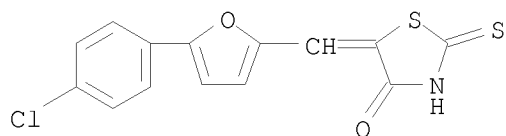
RN 35274-36-3 CAPLUS
CN 4-Thiazolidinone, 5-[[5-(4-nitrophenyl)-2-furanyl]methylene]-2-thioxo-
(CA INDEX NAME)



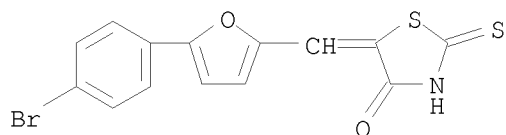
RN 35274-37-4 CAPLUS
CN Benzoic acid, 4-[5-[(4-oxo-2-thioxo-5-thiazolidinylidene)methyl]-2-furanyl]- (CA INDEX NAME)



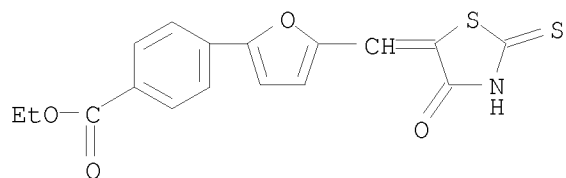
RN 35274-38-5 CAPLUS
CN 4-Thiazolidinone, 5-[[5-(4-chlorophenyl)-2-furanyl]methylene]-2-thioxo-
(CA INDEX NAME)



RN 35274-39-6 CAPLUS
CN 4-Thiazolidinone, 5-[[5-(4-bromophenyl)-2-furanyl]methylene]-2-thioxo-
(CA INDEX NAME)

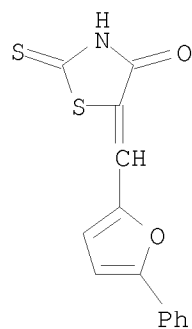


RN 35274-40-9 CAPLUS
CN Benzoic acid, 4-[5-[(4-oxo-2-thioxo-5-thiazolidinylidene)methyl]-2-furanyl]-, ethyl ester (CA INDEX NAME)



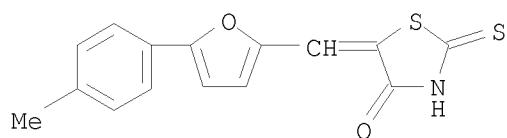
RN 35274-41-0 CAPLUS

CN 4-Thiazolidinone, 5-[(5-phenyl-2-furanyl)methylene]-2-thioxo- (CA INDEX NAME)



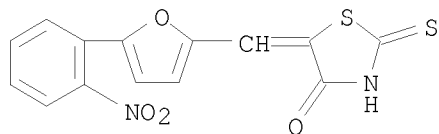
RN 35274-42-1 CAPLUS

CN 4-Thiazolidinone, 5-[[5-(4-methylphenyl)-2-furanyl]methylene]-2-thioxo- (CA INDEX NAME)



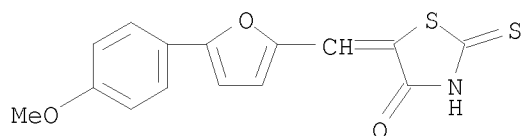
RN 35386-81-3 CAPLUS

CN 4-Thiazolidinone, 5-[[5-(2-nitrophenyl)-2-furanyl]methylene]-2-thioxo- (CA INDEX NAME)



RN 36405-07-9 CAPLUS

CN 4-Thiazolidinone, 5-[[5-(4-methoxyphenyl)-2-furanyl]methylene]-2-thioxo- (CA INDEX NAME)



=> FIL REG

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

8.81

524.59

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-0.80

-1.60

FILE 'REGISTRY' ENTERED AT 08:59:19 ON 02 SEP 2008

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 1 SEP 2008 HIGHEST RN 1045602-82-1

DICTIONARY FILE UPDATES: 1 SEP 2008 HIGHEST RN 1045602-82-1

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TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

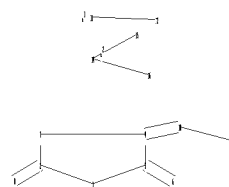
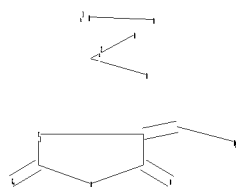
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\STNEXP\Queries\10534919\09_02_08_5.str



```

chain nodes :
6 8 10 11 12 14 15 16 19
ring nodes :
1 2 3 4 5
chain bonds :
2-8 4-10 5-6 10-19 11-12 14-15 14-16
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 2-8 3-4 4-5 4-10 5-6 10-19 11-12 14-15 14-16

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G1:C,O,S,N

G2:O,S,[*1],[*2]

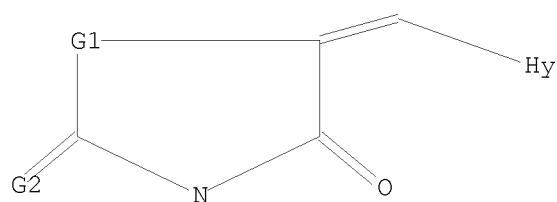
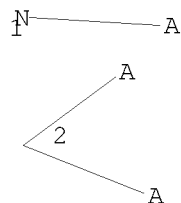
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Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 8:Atom 10:CLASS 11:CLASS
12:CLASS 14:CLASS 15:CLASS 16:CLASS 19:Atom
Generic attributes :
19:
Saturation           : Unsaturated

```

L18 STRUCTURE UPLOADED

=> D
 L18 HAS NO ANSWERS
 L18 STR



G1 C,O,S,N
 G2 O,S,[@1],[@2]

Structure attributes must be viewed using STN Express query preparation.

=> S L18
 SAMPLE SEARCH INITIATED 08:59:36 FILE 'REGISTRY'
 SAMPLE SCREEN SEARCH COMPLETED - 30616 TO ITERATE

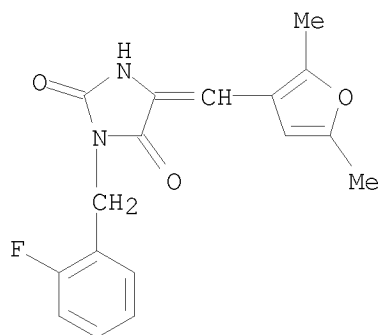
6.5% PROCESSED 2000 ITERATIONS 50 ANSWERS
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 601855 TO 622785
 PROJECTED ANSWERS: 47799 TO 53845

L19 50 SEA SSS SAM L18

=> D SCAN

L19 50 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 2,4-Imidazolidinedione, 5-[(2,5-dimethyl-3-furanyl)methylene]-3-[(2-fluorophenyl)methyl]-
 MF C17 H15 F N2 O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> S L18 FULL

FULL SEARCH INITIATED 08:59:50 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 617712 TO ITERATE

100.0% PROCESSED 617712 ITERATIONS

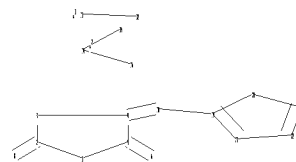
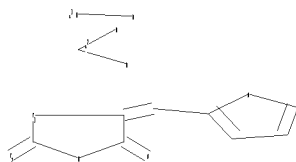
50859 ANSWERS

SEARCH TIME: 00.00.08

L20 50859 SEA SSS FUL L18

=>

Uploading C:\Program Files\STNEXP\Queries\10534919\09_02_08_6.str



chain nodes :

6 8 10 11 12 14 15 16

ring nodes :

1 2 3 4 5 19 20 21 22 23

chain bonds :

2-8 4-10 5-6 10-19 11-12 14-15 14-16

ring bonds :

1-2 1-5 2-3 3-4 4-5 19-20 19-23 20-21 21-22 22-23

exact/norm bonds :

1-2 1-5 2-3 2-8 3-4 4-5 4-10 5-6 10-19 11-12 14-15 14-16 19-20 19-23
20-21 21-22 22-23

G1:C,O,S,N

G2:O,S,[*1],[*2]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 8:Atom 10:CLASS 11:CLASS
12:CLASS 14:CLASS 15:CLASS 16:CLASS 19:CLASS 20:Atom 21:Atom 22:Atom
23:Atom

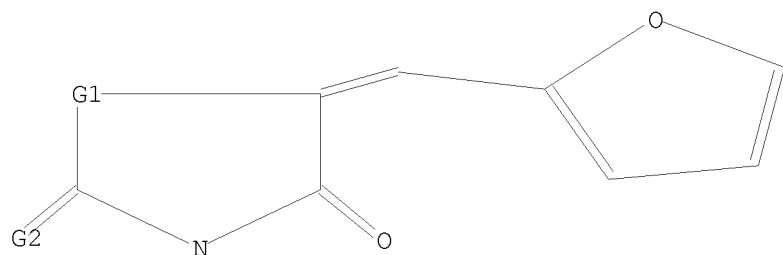
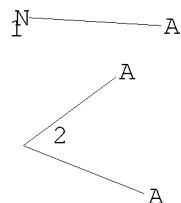
Searched by Jason M. Nolan, Ph.D.

L21 STRUCTURE UPLOADED

=> D

L21 HAS NO ANSWERS

L21 STR



G1 C,O,S,N

G2 O,S,[@1],[@2]

Structure attributes must be viewed using STN Express query preparation.

=> S L21 FULL SUB=L20

FULL SUBSET SEARCH INITIATED 09:01:45 FILE 'REGISTRY'

FULL SUBSET SCREEN SEARCH COMPLETED - 12943 TO ITERATE

100.0% PROCESSED 12943 ITERATIONS

9814 ANSWERS

SEARCH TIME: 00.00.01

L22 9814 SEA SUB=L20 SSS FUL L21

=> S L20 NOT L22

L23 41045 L20 NOT L22

=> FIL CAPLUS

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

221.84

746.43

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

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FILE COVERS 1907 - 2 Sep 2008 VOL 149 ISS 10
FILE LAST UPDATED: 1 Sep 2008 (20080901/ED)

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=> S L23

L24 1233 L23

=> S L22

L25 480 L22

=> S L25 AND COMPOSITION

735831 COMPOSITION

L26 8 L25 AND COMPOSITION

=> D IBIB ABS HITSTR L26 TOT

L26 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:430177 CAPLUS

DOCUMENT NUMBER: 121:30177

ORIGINAL REFERENCE NO.: 121:5497a,5500a

TITLE: Localization of calcium entry through calcium channels in olfactory receptor neurons using a laser scanning microscope and the calcium indicator dyes Fluo-3 and Fura-Red

AUTHOR(S): Schild, D.; Jung, A.; Schultens, H. A.

CORPORATE SOURCE: Physiologisches Inst., Univ. Goettingen, Goettingen, Germany

SOURCE: Cell Calcium (1994), 15(5), 341-8

CODEN: CECADV; ISSN: 0143-4160

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The intracellular calcium concentration [Ca²⁺]_i in olfactory receptor neurons of

Xenopus laevis was imaged with high spatial and temporal resolution. A new method using a mixture of the calcium indicator dyes Fluo-3 and Fura-Red was employed. The fluorescence patterns in two wavelength bands were measured on the emission side of a confocal laser scanning microscope, and the ratio *R* of the fluorescence intensities was taken as an estimate of $[Ca^{2+}]_i$. When the neurons were depolarized by elevating the extracellular potassium concentration $[K^+]_0$ they showed one of three types of responses: a fast

increase

in $[Ca^{2+}]_i$, a slow increase in $[Ca^{2+}]_i$, or no change in $[Ca^{2+}]_i$. The fast increase in $[Ca^{2+}]_i$ took place in the soma compartment. For at least 4 s after the onset of depolarization the calcium distribution in the dendrite remained essentially unchanged. To study the fast increase with high time resolution, line scan images were taken. The neurons were depolarized for brief periods applying a solution containing high $[K^+]$ onto the soma from an application pipet. The fast increase in $[Ca^{2+}]_i$ began with a delay of about 200 ms and went from the resting concentration to about 110 nM above resting concentration. Following the depolarization, recovery from elevated $[Ca^{2+}]_i$ to resting levels had a time constant of about 15 s. The slow response seemed to depend on the removal of $[Na^+]$ from the bath rather than on the elevated $[K^+]$ in the bath. The response was also observed with Cd^{2+} , Ni^{2+} , and Co^{2+} (1.5 mM each) in the bath. The fast increase in $[Ca^{2+}]_i$ upon depolarization was never seen if $R > 0.8$ ($[Ca^{2+}]_i > 300$ nM). For $R < 0.8$, 45% of the cells showed a fast response. Cells that responded with a fast increase in $[Ca^{2+}]_i$ at low resting $[Ca^{2+}]_i$ did not do so for $R > 0.8$. The authors suggest that the physiol. role of calcium entry through calcium channels on the soma of olfactory cells is to decrease the membrane impedance in an activity dependent way by activating a calcium dependent potassium conductance.

IT 149732-62-7, Fura-Red

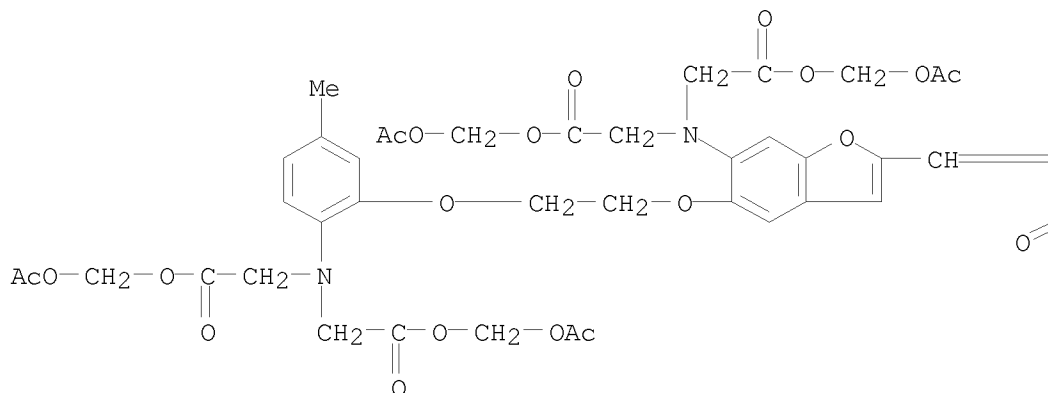
RL: ANST (Analytical study)

(Localization of calcium entry through calcium channels in olfactory receptor neurons using a laser scanning microscope and the calcium indicator dyes Fluo-3 and Fura-Red)

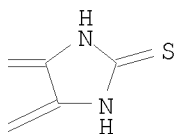
RN 149732-62-7 CAPLUS

CN Glycine, N-[2-[(acetyloxy)methoxy]-2-oxoethyl]-N-[5-[2-[2-[bis[2-[(acetyloxy)methoxy]-2-oxoethyl]amino]-5-methylphenoxy]ethoxy]-2-[(5-oxo-2-thioxo-4-imidazolidinylidene)methyl]-6-benzofuranyl]-, (acetyloxy)methyl ester (CA INDEX NAME)

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L26 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:212943 CAPLUS

DOCUMENT NUMBER: 120:212943

ORIGINAL REFERENCE NO.: 120:37657a,37660a

TITLE: Resting calcium in frog skeletal muscle fibers
estimated with the calcium indicators fluo-3 and fura
red

AUTHOR(S): Harkins, Amy B.

CORPORATE SOURCE: Univ. Pennsylvania, Philadelphia, PA, USA

SOURCE: (1993) 216 pp. Avail.: Univ. Microfilms Int., Order
No. DA9321400

From: Diss. Abstr. Int. B 1993, 54(3), 1253

DOCUMENT TYPE: Dissertation

LANGUAGE: English

AB Unavailable

IT 149732-62-7, Fura red

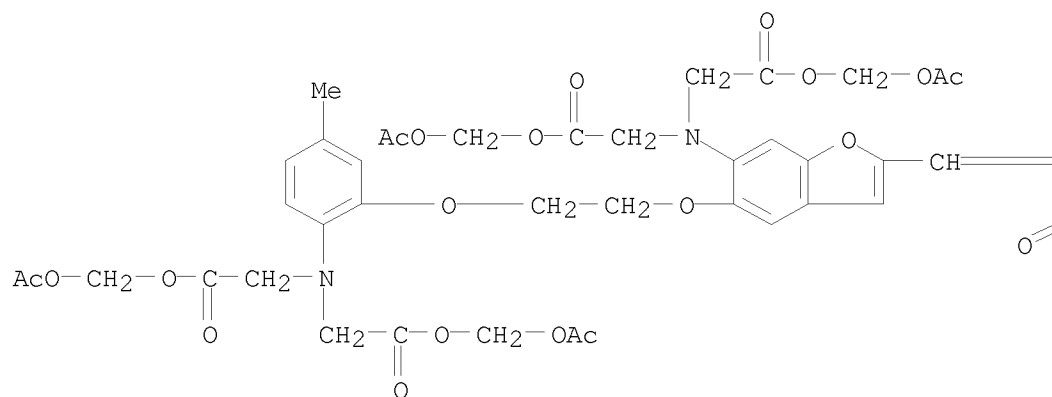
RL: BIOL (Biological study)

(calcium determination in resting muscle by)

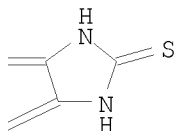
RN 149732-62-7 CAPLUS

CN Glycine, N-[2-[(acetyloxy)methoxy]-2-oxoethyl]-N-[5-[2-[2-[bis[2-
[(acetyloxy)methoxy]-2-oxoethyl]amino]-5-methylphenoxy]ethoxy]-2-[(5-oxo-2-
thioxo-4-imidazolidinylidene)methyl]-6-benzofuranyl]-, (acetyloxy)methyl
ester (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



L26 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1993:534716 CAPLUS

DOCUMENT NUMBER: 119:134716

ORIGINAL REFERENCE NO.: 119:24077a,24080a

TITLE: Ratiometric confocal calcium measurements with visible wavelength indicators in isolated cardiac myocytes

AUTHOR(S): Lipp, P.; Niggli, E.

CORPORATE SOURCE: Dep. Physiol., Univ. Bern, Bern, Switz.

SOURCE: Cell Calcium (1993), 14(5), 359-72

CODEN: CECADV; ISSN: 0143-4160

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A new method for ratiometric Ca^{2+} measurements using indicators with excitation spectra in the visible range of wavelengths is presented. Laser-scanning confocal microscopy was used to record intracellular Ca^{2+} signals with high temporal and spatial resolution in single cardiac myocytes. The patch-clamp technique was applied to load the cells with the fluorescent Ca^{2+} indicators and to follow the membrane currents with the fluorescence signals simultaneously. Intracellular free Ca^{2+} concentration ($[\text{Ca}^{2+}]_i$) was estimated with a ratiometric method. An in vitro calibration procedure was used to convert the fluorescence ratio obtained with two different Ca^{2+} indicators (Fluo-3 and Fura-Red) into Ca^{2+} concns. Fluo-3 showed an increase in fluorescence upon a rise in intracellular Ca^{2+} concentration, while the Fura-Red fluorescence decreased. Since the fluorescence

of Fluo-3 was around 2-fold brighter than the Fura-Red signal the cells were loaded with a 1:2 mixture of the two indicators. The large increase of the fluorescence ratio during a rise in $[\text{Ca}^{2+}]_i$ (up to 4-fold) allowed time-resolved signals to be recorded with this mixture even when monitored in a very small subcellular volume (around $1 \mu\text{m}^3$). Long-lasting continuous recordings of the fluorescence were possible because the dye mixture exhibited no detectable bleaching with illumination periods of up to 30 s. The use of the Fluo-3/Fura-Red ratio method should significantly facilitate and improve quant. measurements of $[\text{Ca}^{2+}]_i$ with high temporal and spatial resolution. Moreover, this approach is especially valuable when

used with confocal microscopes which are usually equipped with lasers in the visible light range. Furthermore, it may be possible to use the same approach with mixts. of other indicators to estimate the concentration of other biol.

important ions/compds. with a ratiometric calibration.

IT 149732-62-7, Fura Red

RL: ANST (Analytical study)

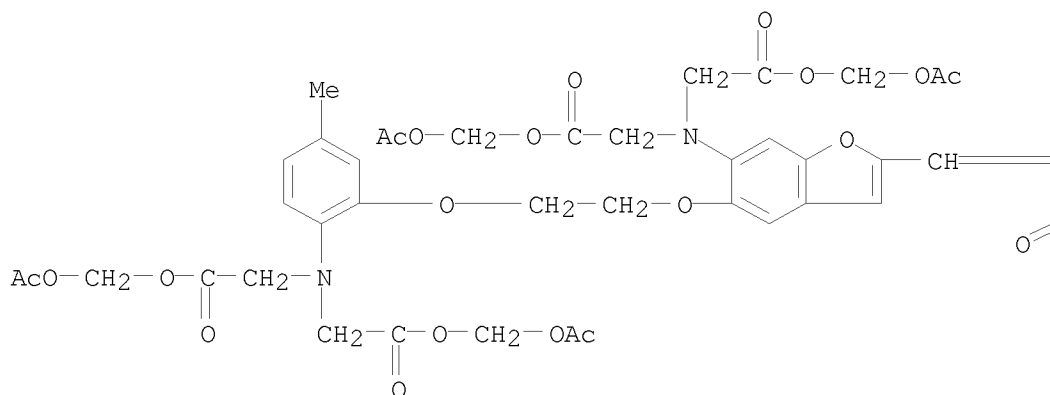
(fluorescence of Fluo-3 and, calcium determination in cardiac myocytes by

radiometric confocal microscopy in relation to)

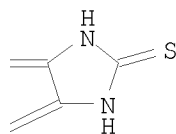
RN 149732-62-7 CAPLUS

CN Glycine, N-[2-[(acetyloxy)methoxy]-2-oxoethyl]-N-[5-[2-[2-[bis[2-[(acetyloxy)methoxy]-2-oxoethyl]amino]-5-methylphenoxy]ethoxy]-2-[(5-oxo-2-thioxo-4-imidazolidinylidene)methyl]-6-benzofuranyl]-, (acetyloxy)methyl ester (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



L26 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1993:467007 CAPLUS

DOCUMENT NUMBER: 119:67007

ORIGINAL REFERENCE NO.: 119:11989a, 11992a

TITLE: Use of fura red as an intracellular calcium indicator in frog skeletal muscle fibers

AUTHOR(S): Kurebayashi, Nagomi; Harkins, A. B.; Baylor, S. M.

CORPORATE SOURCE: Sch. Med., Univ. Pennsylvania, Philadelphia, PA, 19104-6085, USA

SOURCE: Biophysical Journal (1993), 64(6), 1934-60

CODEN: BIOJAU; ISSN: 0006-3495

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Fura red, a fluorescent Ca²⁺ indicator with absorbance bands at visible wavelengths, was injected into intact single muscle fibers that had been stretched to a long sarcomere length (.apprx.3.8 μm) and bathed in a 'high-Ca²⁺' Ringer ([Ca²⁺] = 11.8 mM). From fura red's slow diffusion coefficient in myoplasm, 0.16 (±0.01, SEM) + 10⁻⁶ cm² s⁻¹ (N = 5;

16°C), it is estimated that .apprx.85% of the indicator mols. are bound to muscle constituents of large mol. weight. Binding appears to elevate, by 3- to 4-fold, the indicator's apparent dissociation constant for Ca²⁺ (K_D), which is estimated to be 1.1-1.6 μM in myoplasm. Fura red's myoplasmic absorbance spectrum was used to estimate fr, the fraction of fura red mols. in the Ca²⁺-bound form at rest. In 3 fibers thought to be minimally damaged by the micro-injection, fr was estimated to be 0.15 (±0.01). Thus, resting myoplasmic free [Ca²⁺] ([Ca²⁺]_r) is estimated to be 0.19-0.28 μM. For fibers in normal Ringer solution ([Ca²⁺] = 1.8 mM), at shorter sarcomere length (.apprx.2.7 μM), and containing a nonperturbing concentration of indicator

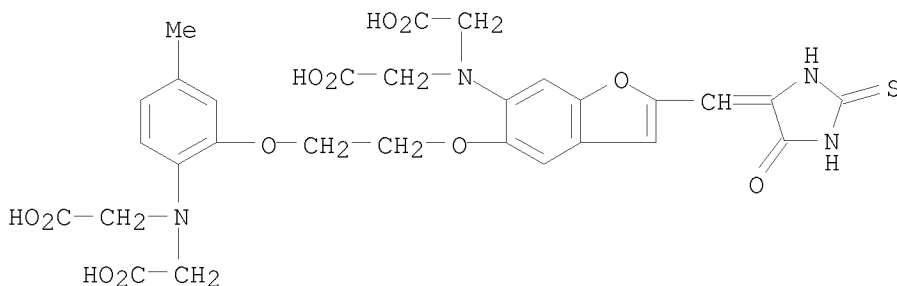
(≤0.2 mM), [Ca²⁺]_r is estimated to be 0.18-0.27 μM. This range is higher than estimated previously in frog fibers with other techniques. In 6 fibers, R, the indicator's fluorescence ratio signal (equal to the emission intensity measured with 420 nm excitation divided by that measured with 480 nm excitation), was measured at rest and following elec. stimulation and compared with absorbance measurements made from the same fiber region. The anal. implies that R_{min} and R_{max} (the values of R that would be measured if all indicator mols. were in the Ca²⁺-free and Ca²⁺-bound states, resp.) were substantially smaller in myoplasm than in calibration solns. lacking muscle proteins. Several methods for estimation of [Ca²⁺]_r from R are analyzed and discussed.

IT 124903-72-6

RL: ANST (Analytical study)
(in calcium determination in muscle fibers)

RN 124903-72-6 CAPLUS

CN Glycine, N-[5-[2-[2-[bis(carboxymethyl)amino]-5-methylphenoxy]ethoxy]-2-[(5-oxo-2-thioxo-4-imidazolidinylidene)methyl]-6-benzofuranyl]-N-(carboxymethyl)- (CA INDEX NAME)



L26 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:51789 CAPLUS

DOCUMENT NUMBER: 112:51789

ORIGINAL REFERENCE NO.: 112:8817a,8820a

TITLE: New tetracarboxylate compounds as fluorescent intracellular calcium indicators

INVENTOR(S): DeMarinis, Robert M.; Katerinopoulos, Haralambos E.; Muirhead, Katharine A.

PATENT ASSIGNEE(S): SmithKline Beckman Corp., USA

SOURCE: U.S., 8 pp.

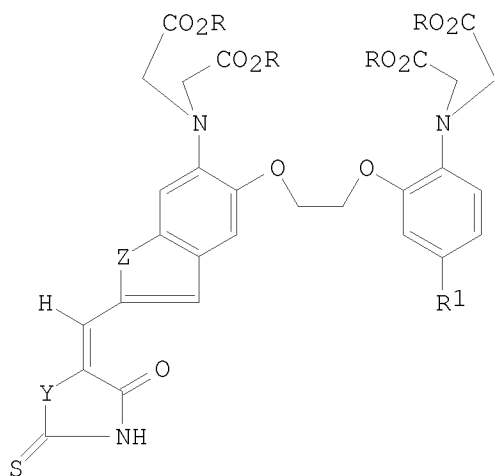
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4849362	A	19890718	US 1988-196654	19880519
EP 342891	A1	19891123	EP 1989-304872	19890515
EP 342891	B1	19940309		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
AT 102619	T	19940315	AT 1989-304872	19890515
ES 2061990	T3	19941216	ES 1989-304872	19890515
JP 02022275	A	19900125	JP 1989-127716	19890519
JP 08013812	B	19960214		
JP 08178850	A	19960712	JP 1995-171874	19950707
JP 2648293	B2	19970827		
PRIORITY APPLN. INFO.:			US 1988-196654	A 19880519
			EP 1989-304872	A 19890515
OTHER SOURCE(S):			MARPAT 112:51789	
GI				

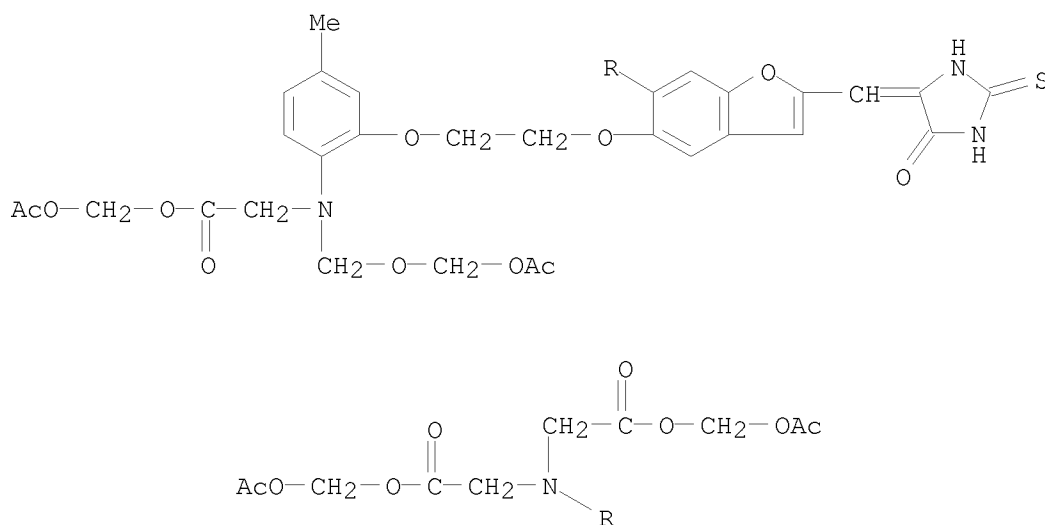


I

- AB Tetracarboxylates I (R = H, AcOCH₂; R₁ = Me, Et; Z = O, S, NH; Y = NH, S) are chelators for Ca²⁺ and are useful as fluorescent indicators for measuring intracellular Ca²⁺ concns. I (R = AcOH₂; R₁ = Me; Z = O; Y = NH) was prepared from 1-(2-amino-4-benzoxylphenoxy)-2-(2'-amino-5'-methylphenoxy)ethane in 9 steps. A10 smooth muscle cells were loaded with indicator dye and analyzed by fluorescence microscopy. Laser output of 100 mW 488 nm was used to excite the fluorescence of Ca²⁺-free tetracarboxylate which was collected using a 640-nm longpass filter. Vasopressin-stimulated increase in intracellular Ca²⁺ caused a decrease in the Ca²⁺-free form of the carboxylate and therefore a decrease in its 488 nm excited fluorescence.
- IT 124903-63-5
RL: ANST (Analytical study)
(fluorescent intracellular calcium indicator)

RN 124903-63-5 CAPLUS

CN Glycine, N-[2-[(acetyloxy)methoxy]-2-oxoethyl]-N-[5-[2-[2-
 [[[acetyloxy)methoxy)methyl][2-[(acetyloxy)methoxy]-2-oxoethyl]amino]-5-
 methylphenoxy]ethoxy]-2-[(5-oxo-2-thioxo-4-imidazolidinylidene)methyl]-6-
 benzofuranyl]-, (acetyloxy)methyl ester (9CI) (CA INDEX NAME)



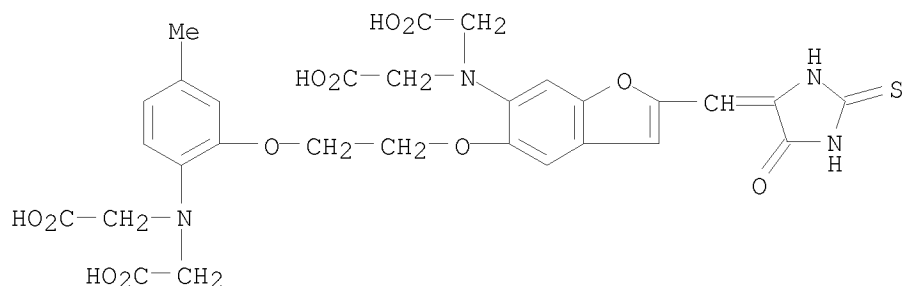
IT 124903-72-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(preparation and reaction of, in preparation of fluorescent intracellular
 calcium
 chelator)

RN 124903-72-6 CAPLUS

CN Glycine, N-[5-[2-[2-[bis(carboxymethyl)amino]-5-methylphenoxy]ethoxy]-2-
 [(5-oxo-2-thioxo-4-imidazolidinylidene)methyl]-6-benzofuranyl]-N-
 (carboxymethyl)- (CA INDEX NAME)



L26 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1981:609650 CAPLUS

DOCUMENT NUMBER: 95:209650

ORIGINAL REFERENCE NO.: 95:34940h,34941a

TITLE: Drug with a cytostatic effect and use of

glycidyl-hydantoin compounds in pharmaceutical composition

INVENTOR(S): Budnowski, Manfred; Fischer, Herbert

PATENT ASSIGNEE(S): Henkel K.-G.a.A., Fed. Rep. Ger.

SOURCE: Ger. Offen., 17 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

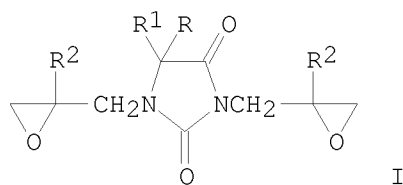
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3003357	A1	19810806	DE 1980-3003357	19800131
EP 33503	A2	19810812	EP 1981-100544	19810126
EP 33503	A3	19820113		
EP 33503	B1	19860910		
R: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
AT 22080	T	19860915	AT 1981-100544	19810126
AU 8166761	A	19810806	AU 1981-66761	19810130
AU 543383	B2	19850418		
JP 56122313	A	19810925	JP 1981-13715	19810131
PRIORITY APPLN. INFO.:				
			DE 1980-3003356	A 19800131
			DE 1980-3003357	A 19800131
			DE 1980-3003404	A 19800131
			AT 1980-1330	A 19800310
			AT 1980-1331	A 19800310
			AT 1980-1365	A 19800312
			AT 1980-1649	A 19800327
			AT 1980-5644	A 19801117
			EP 1981-100544	A 19810126

GI



AB Cytostats, I, where R and R1 are the same or different and H or C1-12 hydrocarbon or closed to a ring, and R2 is H or C1-4 alkyl, were prepared and tested in mice inoculated with leukemia P 388 cells.

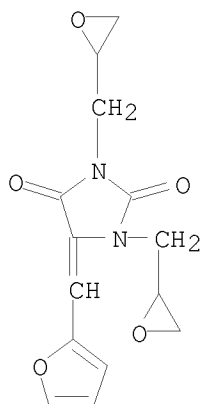
Furfurylidenehydantoin [19628-38-7] and epichlorhydrin [106-89-8] were refluxed with Et4N+Br- catalyst for 4-5 h, cooled to 40-50°, mixed with alkali, and H2O was removed by azeotropic distillation. After stirring 1 h at 40°, NaCl was removed and epichlorhydrin distilled, and the residue was recrystd. from iso-PrOH to give N,N'-diglycidylfurfurylidenehydantoin [79413-01-7] (yield, 65% of theory).

IT 79413-01-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and cytostatic activity of)

RN 79413-01-7 CAPLUS

CN 2,4-Imidazolidinedione, 5-(2-furanylmethylene)-1,3-bis(oxiranylmethyl)-
(9CI) (CA INDEX NAME)

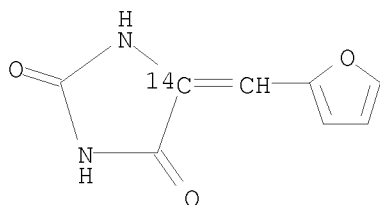


IT 19628-38-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with epichlorhydrin)

RN 19628-38-7 CAPLUS

CN 2,4-Imidazolidinedione-5-14C, 5-(2-furanylmethylene)- (9CI) (CA INDEX NAME)



L26 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1980:41739 CAPLUS

DOCUMENT NUMBER: 92:41739

ORIGINAL REFERENCE NO.: 92:6961a,6964a

TITLE: Pharmaceutical composition useful as
antidote for heavy metal poisoning

INVENTOR(S): Giroux, Eugene L.; Prakash, Nellikunja J.; Schechter,
Paul J.

PATENT ASSIGNEE(S): Merrell Toraude S. A., Fr.

SOURCE: Belg., 13 pp.
CODEN: BEXXAL

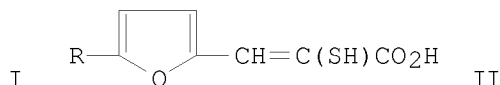
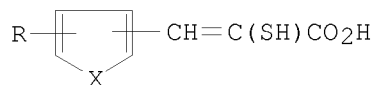
DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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BE 875232	A1	19790716	BE 1979-194334	19790330
US 4169149	A	19790925	US 1978-892187	19780331
ZA 7901524	A	19800827	ZA 1979-1524	19790330
PRIORITY APPLN. INFO.:			US 1978-892187	A 19780331
			US 1977-765420	A2 19770121
OTHER SOURCE(S):	MARPAT 92:41739			
GI				

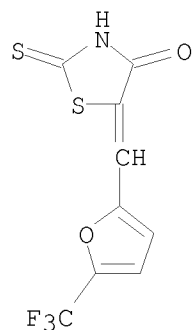


AB Mercaptoacrylic acid I (X = CH:CH, O, S, NH; R = H, Me, Et, OH, OMe, OEt, Cl, Br, F, I, CF₃) were prepared. Thus, 5-trifluoromethylfurfural was treated with rhodamine followed by alkaline hydrolysis to give II (R = CF₃). II (R = H) at 25 mg/kg day protected rat against 1 mg/kg day Cd.

IT 65712-31-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and hydrolysis of)

RN 65712-31-4 CAPLUS

CN 4-Thiazolidinone, 2-thioxo-5-[[5-(trifluoromethyl)-2-furanyl]methylene]-
 (CA INDEX NAME)



L26 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1977:38591 CAPLUS

DOCUMENT NUMBER: 86:38591

ORIGINAL REFERENCE NO.: 86:6119a,6122a

TITLE: Nitrofuran-containing composition and its use as slimicide

INVENTOR(S): Hjelte, Nils; Sandberg, Bo

PATENT ASSIGNEE(S): Rexolin Chemicals AB, Swed.

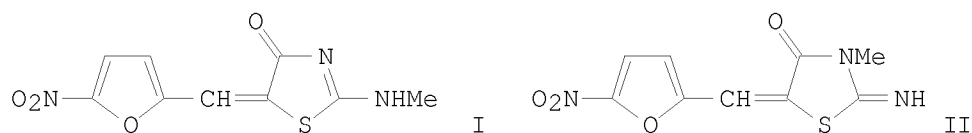
SOURCE: Ger. Offen., 18 pp.
 CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2614798	A1	19761028	DE 1976-2614798	19760406
FI 7600961	A	19761010	FI 1976-961	19760408
SE 7604170	A	19761010	SE 1976-4170	19760408
NO 7601217	A	19761012	NO 1976-1217	19760408
FR 2307081	A1	19761105	FR 1976-10283	19760408
FR 2307081	B3	19790105		
PRIORITY APPLN. INFO.: GI			GB 1975-14640	A 19750409



AB 2-Methylamino-5-(5-nitro-2-furfurylidene)thiazolin-4-one mixture with 3-methyl-2-imino-5-(5-nitro-2-furfurylidene)thiazolidin-4-one [61345-54-8] (I:II = 1:1) is a synergistic bactericide and fungicide suitable for the slime control in paper manufacture. Thus 1.2 g I-II mixture/ton paper controlled bacteria and fungi in 2 machines producing 60 tons of paper daily.

IT 61345-54-8
RL: BIOL (Biological study)
(slimicide for paper manufacture)

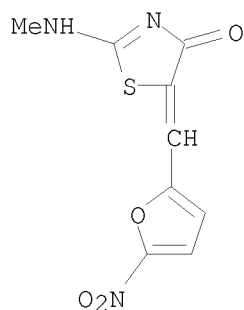
RN 61345-54-8 CAPLUS

CN 4(5H)-Thiazolone, 2-(methylamino)-5-[(5-nitro-2-furanyl)methylene]-, mixt. with 2-imino-3-methyl-5-[(5-nitro-2-furanyl)methylene]-4-thiazolidinone (9CI) (CA INDEX NAME)

CM 1

CRN 25603-06-9

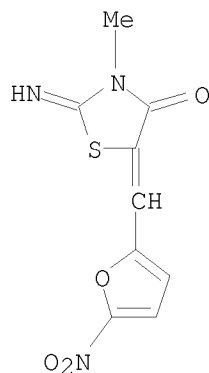
CMF C9 H7 N3 O4 S



CM 2

CRN 25580-69-2

CMF C9 H7 N3 O4 S



=> D IBIB ABS HITSTR L24 1233

L24 ANSWER 1233 OF 1233 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1908:14948 CAPLUS

DOCUMENT NUMBER: 2:14948

ORIGINAL REFERENCE NO.: 2:3229h-i,3230a-g

TITLE: Substituted Rhodaninic Acids and their Aldehyde
Condensation Products (VII)

AUTHOR(S): Andreasch, Rudolph

SOURCE: Monatshefte fuer Chemie (1908), 29, 399-419

CODEN: MOCMB7; ISSN: 0026-9247

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

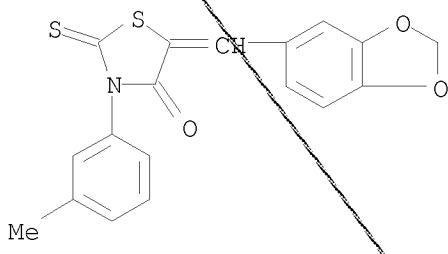
AB cf. Ibid., 24, 499-27, 1211. m-Tolylthiocarbamic acid, prepared by the interaction of m-toluidine, CS₂, and NH₃ is, in the form of its NH₄ salt, allowed to act upon the Et ester of monochloroacetic acid. The resulting v-m-tolylrhodaninic acid (I), m. 148°. In the alcoholic mother liquor is found the ethyl tolyldithiocarbamylacetate, MeC₅H₄.NH.CS.S.CH₂.COOC₂H₅ m. 77°. A number of condensation products were prepared from this tolylrhodaninic acid. With BzH was obtained β-benzylidene-v-m-tolylrhodaninic acid, m. 124°; with salicylic aldehyde, β-o-oxybenzylidene-v-m-tolylrhodaninic acid, m. 220°; with m-nitrobenzaldehyde, β-m-nitrobenzylidene-v-m-tolylrhodaninic acid, m. 234°; with p-dimethyl aminobenzaldehyde, β-dimethyl-p-amidobenzylidene-v-m-tolylrhodaninic acid, m. 140°, a compound which dyes wool a beautiful orange-red; with piperonal, β-methylene-dioxybenzylidene-v-m-tolylrhodaninic acid, m. 178°; with cinnamic aldehyde, β-cinnamylidene-v-m-tolylrhodaninic acid, m. 145-6°. When benzylthiocarbamic acid, prepared by the action of CS₂ upon benzylamine (2 mol.), is allowed to act upon Et monochloroacetate, the final product is v-benzylrhodaninic acid, m. 83°. As condensation products were prepared: with BzH, β-benzylidene-v-benzylrhodaninic acid, m.

219°; with m-nitrobenzaldehyde, β -m-nitrobenzylidene-v-benzylrhodaninic acid, m. 183°; with p-dimethylaminobenzaldehyde, β -dimethyl-p-aminobenzylidene-v-benzylrhodaninic acid, m. 177°. The action of hydrazine in the presence of CS₂ and EtOH gives the hydrazine dithiocarbazinate. The further action of this product upon Et monochloracetate gives v-aminorhodaninic acid (II) m. 92°. From the mother liquor of aminorhodaninic acid was obtained a substance, m. 60°, possibly C₁₀H₁₄O₄N₂S₃. The condensation of aminorhodaninic acid with m-nitrobenzaldehyde gave β -m-nitrobenzylidene-v-aminorhodaninic acid, m. 170°; with p-dimethylaminobenzaldehyde it gave β -dimethyl-p-aminobenzylidene-v-aminorhodaninic acid, m. 266°. In analogy with the action of H₂CO₃ upon the amino acids with the production of the corresponding carbamic acids, the author has substituted CS₂ and obtained from these acids the corresponding dithiocarbamic acids. These latter with Et monochloracetate give substituted rhodaninic acids. Thus, from CS₂ and glycocoll in Ba(OH)₂, to which is finally added a small quantity of EtOH, the compound (III) is formed. The action of Et monochloracetate upon the product gives the yellow Ba rhodaninylacetate (IV). The acid contains 1 H₂O, m. 145°. With aldehydes, this acid condenses in the same manner as did the other rhodaninic acids just described. From BzH was obtained β -benzylidenerhodaninylacetic acid, m. 240°; from m-nitrobenzaldehyde, β -m-nitrobenzylidenerhodaninylacetic acid, m. 270-80°; and from p-dimethylaminobenzylaldehyde, β -dimethyl-p-aminobenzylidenerhodaninylacetic acid, m. and decomposes 235°. Other amino acids such as aniline, aminobenzoic acids, etc., give the corresponding rhodaninic acids. In many cases these products are not crystalline.

IT 340966-32-7P, Rhodanine, 5-piperonylidene-3-m-tolyl-
RL: PREP (Preparation)
(preparation of)

RN 340966-32-7 CAPLUS

CN 4-Thiazolidinone, 5-(1,3-benzodioxol-5-ylmethylene)-3-(3-methylphenyl)-2-thioxo- (CA INDEX NAME)



=> D IBIB ABS HITSTR L24 1232

L24 ANSWER 1232 OF 1233 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1910:8921 CAPLUS

DOCUMENT NUMBER: 4:8921

ORIGINAL REFERENCE NO.: 4:1604b-i,1605a-b

TITLE: Substituted Rhodaninic Acids and their Aldehyde
Condensation Products. VIII

AUTHOR(S): Kaluza, Ludwig

SOURCE: Graz. Manatsh. (1910), 30, 701-26
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Among the substituted acids studied the first under consideration was v-.vphi.-cumylrhodaninic acid (I), prepared by the action of Et monochloroacetate upon NH₄ cumyldithiocarbamate. In this reaction a heavy oil separates and gives, upon standing, small colorless crystals, m. 84°, of ethyl .vphi.-cumyldithiocarbamylacetate, Me₃C₆H₂NHCSSCH₂CO₂Et, an intermediate product in the rhodaninic acid synthesis. Examinations of the oily substance left after separation of the crystals just mentioned showed that the v-.vphi.-cumylrhodaninic acid was present. It could not, however, be obtained pure. A number of its condensation products with aldehydes were prepared. β-Benzylidene-v-.vphi.-cumylrhodaninic acid, C₁₉H₁₇ONS₂, prepared by condensation with BzH, lemon-yellow needles, m. 127°, mol. weight 330.1. β-Methylene-3,4-dioxybenzylidene-v-.vphi.-cumylrhodaninic acid, C₂₀H₁₇O₃NS₂, by condensation with piperonaldehyde; small needles, m. 188°. β-m-nitrobenzylidene-v-.vphi.-cumylrhodaninic acid, C₁₉H₁₆N₂S₂O₃, from m-nitrobenzaldehyde; yellow crystalline powder, m. 224°. β-p-Nitrobenzylidene-v-.vphi.-cumylrhodaninic acid, C₁₉H₁₆N₂S₂O₃, from p-nitrobenzaldehyde; dark yellow powder, m. 230° (decompose). β-Dimethyl-p-aminobenzylidene-v-.vphi.-cumylrhodaninic acid, C₂₁H₂₂ON₂S₂, from β-dimethyl-p-aminobenzaldehyde; dark crystalline powder, m. 192°. β-p-Methoxyl-benzylidene-v-.vphi.-cumylrhodaninic acid, C₂₀H₁₉O₂NS₂, from anisic aldehyde; chrome-yellow plates, m. 174°. The second substituted acid was v-isohexylrhodaninic acid (II) prepared from ClCH₂CO₂Et upon the isohexyl isohexyldithiocarbamate, thick oil, yellow in color. A number of condensation products were prepared: β-benzylidene-v-isohexylrhodaninic acid, C₁₆H₁₉NS₂, from BzH; light yellow needles, m. 87°, mol. weight 282.4. β-m-Nitrobenzylidene-v-isohexylrhodaninic acid, C₁₆H₁₈O₃N₂S₂, from m-nitrobenzaldehyde; light yellow crystals, m. 166-7°. β-p-Nitrobenzylidene-v-isohexylrhodaninic acid, C₁₆H₁₈O₃N₂S₂, from p-nitrobenzaldehyde; brown-yellow crystalline powder, m. 130-1°. β-Methylene-3,4-dioxybenzylidene-v-isohexylrhodaninic acid, C₁₇H₁₉O₃NS₂, from piperonaldehyde; gold-yellow flakes, m. 98°. β-Dimethyl-p-amino-benzylidene-v-isohexylrhodaninic acid, C₁₈H₂₄ON₂S₂, from dimethyl-p-aminobenzaldehyde; red needles, m. 140°. β-o-Hydroxybenzylidene-v-isohexylrhodaninic acid, C₁₆H₁₉O₂NS₂, from salicylic aldehyde, orange-yellow needles, m. 170-2°. β-p-Methoxybenzylidene-v-isohexylrhodaninic acid, C₁₇H₂₁O₂NS₂, from anisic aldehyde; chrome-yellow needles, m. 85°. β-Cinnamylene-v-isohexylrhodaninic acid, C₁₈H₂₁ONS₂, from cinnamic aldehyde, yellow scales, m. 129-31°. The action of Et chlorocarbonate from the isohexylisohexyldithiocarbamate was found to give isohexylisothiocyanate, C₁₇H₁₃NS, yellow oil, b. p. 208-9°. By the action of NH₃ and EtOH it gives a white crystalline isohexylthiourea, C₇H₁₆N₂S, m. 62°. With isohexylamine instead of NH₃ diisohexylthiourea, C₁₃H₂₈N₂S, crystallizing in glancing white leaflets, m. 46°, was obtained. The action of (CN)₂ on isohexylthiourea and the subsequent treatment of this cyanide with HCl gave a monoisohexylthioparabanic acid (III), C₉H₁₄N₂O₂S; light yellow crystals m. 110°, mol. weight 197. When this product is treated with AgNO₃ in EtOH or H₂O, with final mixing, there was extracted by Et₂O a monoisohexylparabanic acid, C₉H₁₄N₂O₃; small white crystals, m. 76°. In a similar manner the diisohexylthiourea was made to give

diisohexylthioparabanic acid, C₁₅H₂₆O₂N₂S; lemon-yellow needles, m. 40°. This in turn gave diisohexylparabanic acid, which however could not be prepared pure or in crystalline form.

IT 859960-24-0P, Rhodanine, 5-piperonylidene-3-pseudocumyl-

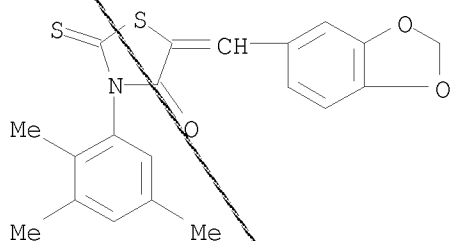
860757-30-8P, Rhodanine, 3-isohexyl-5-piperonylidene-

RL: PREP (Preparation)

(preparation of)

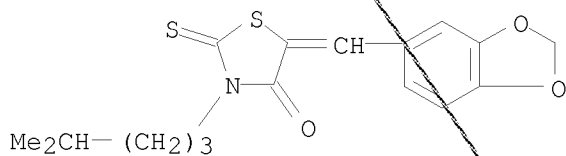
RN 859960-24-0 CAPLUS

CN 4-Thiazolidinone, 5-(1,3-benzodioxol-5-ylmethylene)-2-thioxo-3-(2,3,5-trimethylphenyl)- (CA INDEX NAME)



RN 860757-30-8 CAPLUS

CN 4-Thiazolidinone, 5-(1,3-benzodioxol-5-ylmethylene)-3-(4-methylpentyl)-2-thioxo- (CA INDEX NAME)



=> D IBIB ABS HITSTR L24 1231

L24 ANSWER 1231 OF 1233 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1911:9676 CAPLUS

DOCUMENT NUMBER: 5:9676

ORIGINAL REFERENCE NO.: 5:1756b-i,1757a

TITLE: Substituted Rhodanines and their Aldehyde Condensation Products. X

AUTHOR(S): Andreasch, Rudolf

SOURCE: Monatshefte fuer Chemie (1911), 31, 785-95

CODEN: MOCMB7; ISSN: 0026-9247

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB cf. C. A., 2, 3229. Dithiocarbaminoacetic acid HS₂CNHCH₂CO₂H, is best prepared from aminoacetic acid, CS₂ and NH₃, in dilute alc., the product consists of diammonium dithiocarbaminoacetate; white needles with 1H₂O, m. 110° (gas evolution). Yield, about 80%. In a similar manner, alanine forms diammonium α-dithiocarbaminopropionate, NH₄S₂CNHCHMeCO₂NH₄; long needles with 1H₂O, m. 128-9° (decompose and gas evolution). When treated with HCl, or H₂SO₄ and Et₂O it gives

α -rhodaninepropionic acid formula (I) below; warty crystals from alc., m. 127°. The above condensation may also be realized by the use of KOH, or Ba(OH)₂ in place of NH₃. β -Benzylidene- α -rhodaninepropionic acid (II), from (I) and BzH, in Et₂O; light yellow needles, or warty aggregates from alc., m. 191°.

β -p-Dimethylaminobenzylidene- α -rhodaninepropionic acid (III), from (I) and p-dimethyl-aminobenzaldehyde; needles, or crusts resembling CrO₃ in color, m. 210-20°. It dyes the skin, wool and silk orange-red, but the colors are not very fast towards light.

β -p-Hydroxybenzylidene- α -rhodaninepropionic acid (IV), from (I) and p-hydroxybenzaldehyde; light chrome-yellow needles or crusts, softens 190°, m. 205-10°.

β -Methylenedioxybenzylidene- α -rhodaninepropionic acid, (V), from (I) and piperonaldehyde in AcOH; orange-yellow warts from alc. or Et₂O, m. 197-9°. When glycylglycine hydrochloride is treated with CS₂ and aqueous NH₃ it appears to form the di-NH₄ dithiocarbamate, NH₄S₂CNHCH₂CONHCH₂CO₂NH₄. It was not purified but was heated with chloroacetic ester and the product acidified and extracted with Et₂O. The resulting compound consists of rhodanineglycylglycine (IV); yellow syrup. With BzH, in AcOH, it forms β -benzylidenerhodanineglycylglycine (VII); greenish yellow scales, or needles, softens 180°, m. 190°. The rhodanines from asparagine, aspartic and glutamic acids and synthetic leucine, both optically active and inactive, are all oils, as are likewise their condensation products with aldehydes. As these oils decompose when heated the compds. in question could not be purified.

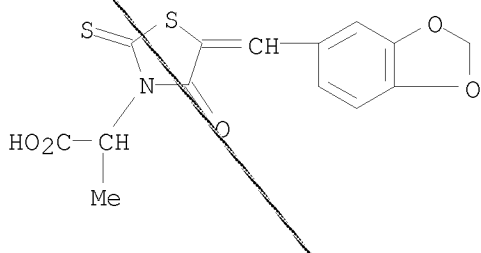
IT 300812-43-5P, 3-Thiazolidineacetic acid, 4-keto- α -methyl-5-piperonylidene-2-thio-

RL: PREP (Preparation)

(preparation of)

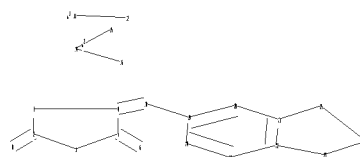
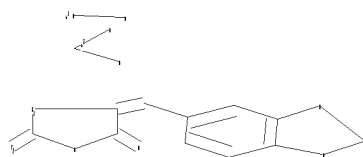
RN 300812-43-5 CAPLUS

CN 3-Thiazolidineacetic acid, 5-(1,3-benzodioxol-5-ylmethylene)- α -methyl-4-oxo-2-thioxo- (CA INDEX NAME)



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chain nodes :

6 8 10 11 12 14 15 16

ring nodes :

1 2 3 4 5 19 20 21 22 23 24 25 26 27

chain bonds :

2-8 4-10 5-6 10-19 11-12 14-15 14-16

ring bonds :

1-2 1-5 2-3 3-4 4-5 19-20 19-24 20-21 21-22 21-25 22-23 22-27 23-24
25-26 26-27

exact/norm bonds :

1-2 1-5 2-3 2-8 3-4 4-5 4-10 5-6 10-19 11-12 14-15 14-16 21-25 22-27
25-26 26-27

normalized bonds :

19-20 19-24 20-21 21-22 22-23 23-24

G1:C,O,S,N

G2:O,S,[*1],[*2]

Match level :

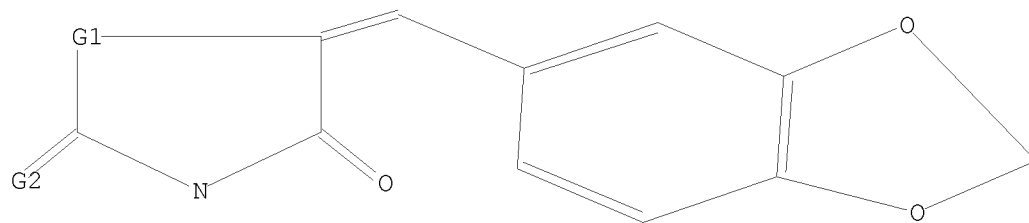
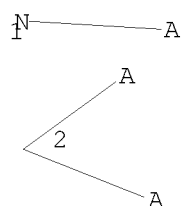
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 8:Atom 10:CLASS 11:CLASS
12:CLASS 14:CLASS 15:CLASS 16:CLASS 19:Atom 20:Atom 21:Atom 22:Atom
23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom

L27 STRUCTURE UPLOADED

=> D

L27 HAS NO ANSWERS

L27 STR



G1 C,O,S,N

G2 O,S,[@1],[@2]

Structure attributes must be viewed using STN Express query preparation.

=> S L27 FULL SUB=L23

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SUBSET SEARCH INITIATED 09:10:12 FILE 'REGISTRY'

FULL SUBSET SCREEN SEARCH COMPLETED - 2970 TO ITERATE

100.0% PROCESSED

2970 ITERATIONS

2111 ANSWERS

Searched by Jason M. Nolan, Ph.D.

SEARCH TIME: 00.00.01

L28 2111 SEA SUB=L23 SSS FUL L27

SUBSET IS IGNORED AS A SCOPE FOR THIS SEARCH

L29 164 L28

=> D IBIB ABS HITSTR L29 164

L29 ANSWER 164 OF 164 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1908:14948 CAPLUS

DOCUMENT NUMBER: 2:14948

ORIGINAL REFERENCE NO.: 2:3229h-i,3230a-g

TITLE: Substituted Rhodaninic Acids and their Aldehyde
Condensation Products (VII)

AUTHOR(S): Andreasch, Rudolph

SOURCE: Monatshefte fuer Chemie (1908), 29, 399-419

CODEN: MOCMB7; ISSN: 0026-9247

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB cf. Ibid., 24, 499-27, 1211. m-Tolylthiocarbamic acid, prepared by the interaction of m-toluidine, CS₂, and NH₃ is, in the form of its NH₄ salt, allowed to act upon the Et ester of monochloroacetic acid. The resulting v-m-tolylrhodaninic acid (I), m. 148°. In the alcoholic mother liquor is found the ethyl tolyldithiocarbamylacetate, MeC₅H₄.NH.CS.S.CH₂.COOC₂H₅ m. 77°. A number of condensation products were prepared from this tolylrhodaninic acid. With BzH was obtained β-benzylidene-v-m-tolylrhodaninic acid, m. 124°; with salicylic aldehyde, β-o-oxybenzylidene-v-m-tolylrhodaninic acid, m. 220°; with m-nitrobenzaldehyde, β-m-nitrobenzylidene-v-m-tolylrhodaninic acid, m. 234°; with p-dimethyl aminobenzaldehyde, β-dimethyl-p-amidobenzylidene-v-m-tolylrhodaninic acid, m. 140°, a compound which dyes wool a beautiful orange-red; with piperonal, β-methylene-dioxybenzylidene-v-m-tolylrhodaninic acid, m. 178°; with cinnamic aldehyde, β-cinnamylidene-v-m-tolylrhodaninic acid, m. 145-6°. When benzyldithiocarbamic acid, prepared by the action of CS₂ upon benzylamine (2 mol.), is allowed to act upon Et monochloroacetate, the final product is v-benzylrhodaninic acid, m. 83°. As condensation products were prepared: with BzH, β-benzylidene-v-benzylrhodaninic acid, m. 219°; with m-nitrobenzaldehyde, β-m-nitrobenzylidene-v-benzylrhodaninic acid, m. 183°; with p-dimethylaminobenzaldehyde, β-dimethyl-p-aminobenzylidene-v-benzylrhodaninic acid, m. 177°. The action of hydrazine in the presence of CS₂ and EtOH gives the hydrazine dithiocarbazinate. The further action of this product upon Et monochloroacetate gives v-aminorhodaninic acid (II) m. 92°. From the mother liquor of aminorhodaninic acid was obtained a substance, m. 60°, possibly C₁₀H₁₄O₄N₂S₃. The condensation of aminorhodaninic acid with m-nitrobenzaldehyde gave β-m-nitrobenzylidene-v-aminorhodaninic acid, m. 170°; with p-dimethylaminobenzaldehyde it gave β-dimethyl-p-aminobenzylidene-v-aminorhodaninic acid, m. 266°. In analogy with the action of H₂CO₃ upon the amino acids with the production of the corresponding carbamic acids, the author has substituted CS₂ and obtained from these

acids the corresponding dithiocarbamic acids. These latter with Et monochloracetate give substituted rhodaninic acids. Thus, from CS₂ and glycocoll in Ba(OH)₂, to which is finally added a small quantity of EtOH, the compound (III) is formed. The action of Et monochloracetate upon the product gives the yellow Ba rhodaninylacetate (IV). The acid contains 1 H₂O, m. 145°. With aldehydes, this acid condenses in the same manner as did the other rhodaninic acids just described. From BzH was obtained β -benzylidenerhodaninylacetic acid, m. 240°; from m-nitrobenzaldehyde, β -m-nitrobenzylidenerhodaninylacetic acid, m. 270-80°; and from p-dimethylaminobenzylaldehyde, β -dimethyl-p-aminobenzylidenerhodaninylacetic acid, m. and decomposes 235°. Other amino acids such as aniline, aminobenzoic acids, etc., give the corresponding rhodaninic acids. In many cases these products are not crystalline.

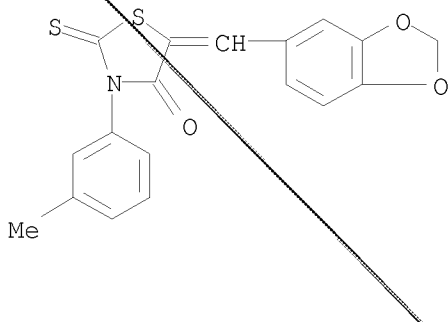
IT 340966-32-7P, Rhodanine, 5-piperonylidene-3-m-tolyl-

RL: PREP (Preparation)

(preparation of)

RN 340966-32-7 CAPLUS

CN 4-Thiazolidinone, 5-(1,3-benzodioxol-5-ylmethylene)-3-(3-methylphenyl)-2-thioxo- (CA INDEX NAME)



=> S L24 NOT L29

L30 1069 L24 NOT L29

=> D IBIB ABS HITSTR L30 1069

L30 ANSWER 1069 OF 1069 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1924:16150 CAPLUS

DOCUMENT NUMBER: 18:16150

ORIGINAL REFERENCE NO.: 18:2166d-e

TITLE: Use of rhodanine in organic syntheses. IV. Indole- and furylpyrrolacemic acids

AUTHOR(S): Granacher, Ch.; Gero, M.; Schelling, V.

SOURCE: Helvetica Chimica Acta (1924), 7, 575-8

CODEN: HCACAV; ISSN: 0018-019X

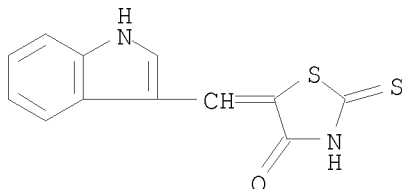
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. C. A. 17, 2424. β -Indolalrhodanine, glistening brown leaflets, which gradually decompose above 200°. Heated with 10% KOH for 1-2 hrs., it gives β -indole- α -sulfhydryl-acrylic acid, orange-yellow, decomp. 190°. The NH₄OH solution gives with FeCl₃ a typical dark green color. With concentrated NH₄OH on the H₂O bath this gives β -indole-pyrrolacemic acid (Ellinger and Matsuoka, C. A. 16, 951). Furylsulfhydrylacrylic acid cannot be directly changed into

furylpyrrolic acid, m. 131°, by heating with NH₃ but is transformed into the oxime and this is decomposed by H₂SO₄. The acid is very unstable and in a few days gives a greenish yellow or dark resinous mass.

IT 73855-59-1P, Rhodanine, 5-(3-indylmethylene)-
RL: PREP (Preparation)
(preparation of)
RN 73855-59-1 CAPLUS
CN 4-Thiazolidinone, 5-(1H-indol-3-ylmethylene)-2-thioxo- (CA INDEX NAME)



=> D IBIB ABS HITSTR L30 1068

L30 ANSWER 1068 OF 1069 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1925:4555 CAPLUS

DOCUMENT NUMBER: 19:4555

ORIGINAL REFERENCE NO.: 19:637g-i

TITLE: Hydantoins. XLIII. Synthesis of the
polypeptide-hydantoin: "hydantoin-3-acetic acid."

AUTHOR(S): Johnson, T. B.; Renfrew, Alice G.

SOURCE: Journal of the American Chemical Society (1925), 47,
240-5

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB SCNCH₂CO₂Et (I) (for which a practical method of preparation is given) reacts with EtOH after heating 9 hrs. at 125° to give di-Et thioncarbamacetate, b₁₀ 135-40° (with considerable decomposition). I and H₂NCH₂CO₂Et in anhydrous Et₂O give a mixture of di-Et thioureadiacetate (II), m. 85-7°, and the mono-Et ester, m. 96°, separated from II by its greater solubility in 50% AcOH. Either ester with HCl yields 2-thiohydantoin-3-acetic acid (III), yellow, m. 210-2° to a yellow oil; the alkali solution is wine-red. This is desulfurized by ClCH₂CO₂H, giving hydantoin-3-acetic acid, m. 190-1°. III is also obtained in good yield from I and H₂NCH₂CO₂H after repeated evaporation with HCl.

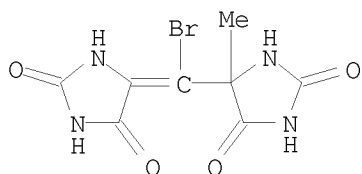
IT 871893-67-3P, Hydantoin, 5-[bromo(2,3,4,5-tetrahydro-2,5-diketo-4-methyl-4-imidazolyl)methylene]-

RL: PREP (Preparation)

(preparation of)

RN 871893-67-3 CAPLUS

CN Hydantoin, 5-[bromo(2,3,4,5-tetrahydro-2,5-diketo-4-methyl-4-imidazolyl)methylene]- (2CI) (CA INDEX NAME)



=> D IBIB ABS HITSTR L30 1067

L30 ANSWER 1067 OF 1069 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1925:4556 CAPLUS

DOCUMENT NUMBER: 19:4556

ORIGINAL REFERENCE NO.: 19:637i

TITLE: Hydantoins. XLIV. Pyvuril and dipyruvic triureide

AUTHOR(S): Davidson, David

SOURCE: Journal of the American Chemical Society (1925), 47, 255-9

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

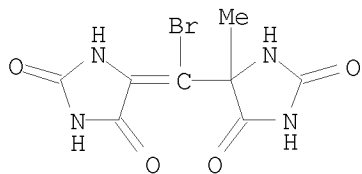
AB Pyvuril (Grimaux, Ann. chim. phys. [5] 11, 367) reacts with 1 mol. Br in AcOH to give CO(NH₂)₂ and bromopyruvic ureide and with 2 mols. to give CO(NH₂)₂ and the di-Br derivative This is analogous to the action of HNO₃. HI gives 5-methylhydantoin, which confirms the intermediate existence of pyruvic monoureide; this has not been isolated on account of its reactivity, undergoing polymerization to dipyruvic acid. Concentrated H₂SO₄ gives dipyruvic ureide, m. 290°, whose Br derivative, C₈H₇BrN₄O₄, m. 265° (decomposition). Similar results were obtained with dipyruvic triureide.

IT 871893-67-3P, Hydantoin, 5-[bromo(2,3,4,5-tetrahydro-2,5-diketo-4-methyl-4-imidazolyl)methylene]-

RL: PREP (Preparation)
(preparation of)

RN 871893-67-3 CAPLUS

CN Hydantoin, 5-[bromo(2,3,4,5-tetrahydro-2,5-diketo-4-methyl-4-imidazolyl)methylene]- (2CI) (CA INDEX NAME)



=> D IBIB ABS HITSTR L30 1066

L30 ANSWER 1066 OF 1069 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1925:6026 CAPLUS

DOCUMENT NUMBER: 19:6026

ORIGINAL REFERENCE NO.: 19:830a-f
TITLE: The metabolism of tryptophan. I. The synthesis of racemic bz-3-methyltryptophan
AUTHOR(S): Robson, Wm.
SOURCE: Journal of Biological Chemistry (1924), 62, 495-514
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

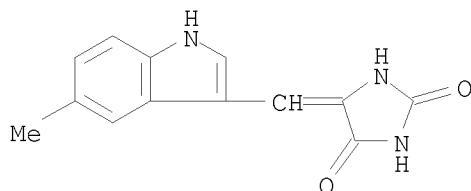
AB A good yield of p-tolylhydrazine is to be obtained only if the temperature is kept at 0-2°. This was then combined with AcCO₂H to yield pyruvic acid p-tolylhydrazone, m. 159° (yield 88%), which was treated in 7 parts absolute EtOH at 65-70° with a rapid stream of dry HCl. After 2 hrs. the mixture was allowed to cool and was then poured into a large volume of H₂O. After filtering and drying, it was distilled 2-Carboxy-5-methylindole, b_{4.0} 236°, m. 163° (yield 60%). This was hydrolyzed with EtOH-KOH, the acid liberated by acidification and extracted with Et₂O. The Et₂O solution was dried with Na₂SO₄, filtered and then treated with a rapid stream of dry NH₃. NH₄ 5-methylindole-2-carboxylate began to sep. as a light yellow powder almost immediately. After saturation, the mixture was allowed to stand 2 or 3 hrs. and was then filtered. Ten g. of the dry NH₄ salt were then placed in a 1-l. flask and heated, under a long air condenser, at 230-40° for 30 min. After distillation in steam, 5-methylindole, m. 58.5°, separated, yield 3.9 g. This could be converted into 5-methylindole-3-aldehyde, m. 148°, by Ellinger and Flamand's method (C. A. 1, 2480), with a yield of 1.2 g. from 9 g. methylindole, and a recovery of 4.6 g. unchanged methylindole and the formation of 3-chloro-6-methylquinoline, m. 85.5°, has an odor resembling lilac. A 1.15 g. yield of a purer 5-methylindole-3-aldehyde, m. 151°, was obtained by the method of Majima and Kotake (C. A. 17, 1017) from 6.5 g. methylindole but no unchanged methylindole was recovered. In a 3rd method, 2-carbethoxy-5-methylindole was converted into 2-carboxy-5-methylindole-3-aldehyde, m. 189°, by Adams and Levine's modification of the Gatterman method (C. A. 17, 3867). On hydrolysis with 40% NaOH for 15 min. and reacidification, 2-carboxy-5-methylindole-3-aldehyde was precipitated. After solution in NH₄OH and repptn. this turned brown at 235° and decomposed violently at 254-5°. Attempts at the preparation of 5-methylindole-3-aldehyde from this were unsuccessful. 5-Methylindolalhydantoin, from the 3-aldehyde, hydantoin, NaOAc and Ac₂O (cf. Majima and Kotake, loc. cit.) m. 295-8°. This in 0.5 NaOH was reduced with Na-Hg to 5-methylindolylhydantylmethane, m. 206-7°. This was then hydrolyzed with Ba(OH)₂, the Ba precipitated with H₂SO₄, and the bz-3-methyltryptophan, precipitated with HgSO₄. The precipitate was filtered out, decomposed in dilute Ba(OH)₂ with H₂S, filtered, the Ba removed with H₂SO₄ and the filtrate evaporated in vacuo. EtOH precipitated a semicryst. mass, which was redissolved in H₂O, repptd. with EtOH, and recrystd. from 50% EtOH. Yield 0.39 g. from 1.2 g. of the hydantylmethane. bz-3-Methyltryptophan, m. 259-63°, gives a beautiful purple with the Hopkins-Cole reagent; a purple color, which may be extracted with BuOH, with Br₂-H₂O; a strong reaction with triketohydrindene hydrate and is very bitter.

IT 857767-36-3P, Hydantoin, 5-(5-methyl-3-indylmethylene)-
RL: PREP (Preparation)
(preparation of)

RN 857767-36-3 CAPLUS

CN 2,4-Imidazolidinedione, 5-[(5-methyl-1H-indol-3-yl)methylene]- (CA INDEX

NAME)



=> D IBIB ABS HITSTR L30 1065

L30 ANSWER 1065 OF 1069 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1925:7147 CAPLUS

DOCUMENT NUMBER: 19:7147

ORIGINAL REFERENCE NO.: 19:973b-d

TITLE: Hydantoin. XLV. Dipyrucic ureide

AUTHOR(S): Davidson, David; Johnson, T. B.

SOURCE: Journal of the American Chemical Society (1925), 47, 561-7

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

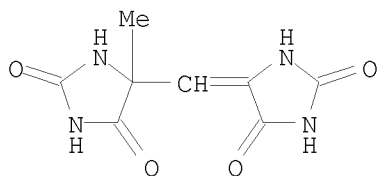
AB cf. C. A. 19, 637. Dipyrucic ureide (I), $\text{HN.CO.NH.CO.C:CHCMe.CO.NH.CO.NH}$, may be obtained from pyruvil or dipyrucic triureide by the action of H_2SO_4 , HBr or HCl ; 6.4 g. result by adding to 10 g. pyruvic acid and 15 g. $\text{CO(NH}_2)_2$ in 15 cc. concentrated HCl , after 36 hrs., 17 g. concentrated H_2SO_4 . Reduction with Pt and H in glacial AcOH gives the hydro derivative, $\text{C}_8\text{H}_{10}\text{O}_4\text{N}_4$, m. about 300° (decomposition). I (4.5 g.) in 25 cc. glacial AcOH , treated on the H_2O bath with 2 cc. Br , gives about 5 g. Br derivative (II), $\text{C}_8\text{H}_7\text{O}_4\text{N}_4\text{Br}$, decomp. about $265-70^\circ$. Warming I with Br water gives bromomethenyl-5'-[5'-methyl]hydantoin-5-hydantoic acid, crystallizing with $3\text{H}_2\text{O}$,

which is lost on the hot plate, giving feathery needles of the anhydrous compound. Heated on the steam bath with concentrated H_2SO_4 , II is formed. Br water reacts with II to give the di- Br derivative, hexagonal plates, m. about 250° (decomposition); soluble in about 17 parts boiling H_2O . Concentrated HNO_3 gives with I nitropyrucic ureide and parabanic acid.

IT 861323-75-3P, Hydantoin, 5-[(2,3,4,5-tetrahydro-2,5-diketo-4-methyl-4-imidazolyl)methylene]- 871893-67-3P, Hydantoin, 5-[bromo(2,3,4,5-tetrahydro-2,5-diketo-4-methyl-4-imidazolyl)methylene]-
 RL: PREP (Preparation)
 (preparation of)

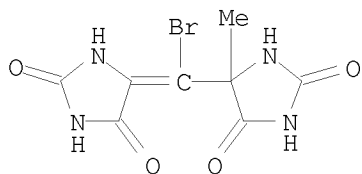
RN 861323-75-3 CAPLUS

CN Hydantoin, 5-[(2,3,4,5-tetrahydro-2,5-diketo-4-methyl-4-imidazolyl)methylene]- (2CI) (CA INDEX NAME)



RN 871893-67-3 CAPLUS

CN Hydantoin, 5-[bromo(2,3,4,5-tetrahydro-2,5-diketo-4-methyl-4-imidazolyl)methylene]- (2CI) (CA INDEX NAME)



=> D IBIB ABS HITSTR L30 1064

L30 ANSWER 1064 OF 1069 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1928:4734 CAPLUS

DOCUMENT NUMBER: 22:4734

ORIGINAL REFERENCE NO.: 22:588f-i,589a

TITLE: Some pyrrole derivatives. II

AUTHOR(S): Kuster, Wm.; Koppenhofer, G.

SOURCE: Z. physiol. Chem. (1927), 172, 126-37

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Synthetic pyrrolamino acids are of interest in connection with the study of the prosthetic group of the blood pigment. The condensation of formylpyrrole derivs. with diketopiperazine, followed by hydrogenation and opening of the anhydride ring, affords a method for preparing alanine derivs. of this type. 2,2-Di[3,5-dimethyl-4-carbethoxypyrral]-2,5-diketopiperazine (I), red crystals, m. 268-9°, was obtained in 60% yield by refluxing a mixture of 3,5-dimethyl-4-carbethoxy-2-formylpyrrole and glycine anhydride with AcOH and NaOAc. Its di-Me derivative, red crystals, m. 156°, was prepared by treating the Ag salt of I with MeI. Reduction of I in EtOH by Al-Hg and neutralization with dilute H₂SO₄ gave an almost quant. yield of colorless 2,2-di[3,5-dimethyl-4-carbethoxypyrrylmethyl]-2,5-diketopiperazine (II), m. 122°. Attempts to prepare a monopyrral derivative of diketopiperazine were unsuccessful, both CH₂ groups of the latter being equally reactive. Hydrolysis of II by Ba(OH)₂ gave 55% of β-[3,5-dimethyl-4-carbethoxypyrryl-2]-alanine (III), which decomp. 180-6° and does not form a Cu salt. Another method of preparing III consists in condensing the formylpyrrole with rhodanin, hydrolyzing the rhodanin ring, converting the resulting thioketonic acid into the oxime and reducing the latter. 3,6-Dimethyl-4-carbethoxy-2-pyrralrhodanin (IV), red needles, m. 253-5°, was obtained in 80% yield by refluxing the formylpyrrole and rhodanin with AcOH and NaOAc; phenylhydrazone, red needles, m.

272-5° (decomposition). Hydrolysis of IV by Ba(OH)₂ converted it into 3,5-dimethyl-4-carbethoxy-2-pyrrylthiopyruvic acid (V), decomp. 196°; oxime, m. 218°. Reduction of the oxime by Na-Hg in the presence of lactic acid gave 62% of III. Hydrolysis of the CS group in V by heating in a sealed tube with ClCH₂CO₂H converted it into 3,5-dimethyl-4-carbethoxy-2-pyrrylpyruvic acid, m. 192°. 1-Phenyl-2,5-dimethyl-3-carbethoxypyrrole was condensed with aminoacetal by heating with concentrated HCl, forming

di[1-phenyl-2,5-dimethyl-3-carbethoxy-4-pyrryl]-β-aminoethane, m. 246°. Similarly, 1-phenyl-2,5-dimethyl-4-carbethoxypyrrole with CH₂O and HCl yielded di[1-phenyl-2,5-dimethyl-4-carbethoxy-3-pyrryl]methane, m. 102°.

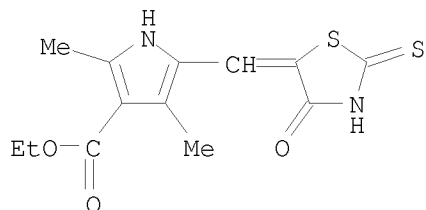
IT 856076-91-0P, 3-Pyrrolicarboxylic acid, 5-(2,3-dihydro-4-keto-2-thioketo-5(4)-thiazylidenemethyl)-2,4-dimethyl-, ethyl ester

RL: PREP (Preparation)

(preparation of)

RN 856076-91-0 CAPLUS

CN INDEX NAME NOT YET ASSIGNED



=> D IBIB ABS HITSTR L30 1063

L30 ANSWER 1063 OF 1069 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1938:14713 CAPLUS

DOCUMENT NUMBER: 32:14713

ORIGINAL REFERENCE NO.: 32:2114h-i,2115a-c

TITLE: Synthesis of r-6-methoxytryptophan and of harmine, with a note on the action of acetaldehyde on tryptophan

AUTHOR(S): Harvey, Douglas G.; Robson, Wm.

SOURCE: Journal of the Chemical Society (1938) 97-101

CODEN: JC SOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal

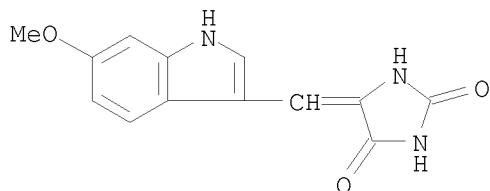
LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 32:14713

AB Details are given of the preparation of the following intermediates: o-nitro-p-cresol, o-nitro-p-tolyl Me ether, the K derivative of Et o-nitro-p-methoxyphenyl-pyruvate, NH₄ 6-methoxyindole-2-carboxylate, 6-methoxyindole and 6-methoxyindole-3-aldehyde (I) (the last being accompanied with some 3-chloro-7-methoxy-quinoline). Heating 3.5 g. I, 2.3 g. hydantoin and 10 ml. piperidine under reflux for 35 min. gives 3.7 g. 5-(6'-methoxyindolal)-hydantoin (II), yellow, m. 311-15°; it gives, when heated with Ehrlich's reagent, a very pale pink color which fades rapidly on cooling. Reduction of 1 g. of II in pyridine with H₂S by heating at 100° for 70 hrs. gives 0.45 g. of 5-(6'-

methoxyindolylmethyl)hydantoin, m. 220° (50% yield on basis of recovered II); cleavage by heating with dilute NH₄OH at 100-10° for 72 hrs. gives 60% of 6-methoxytryptophan (III), m. 263-8°, decomp. 274°; it has an intensely sweet taste, gives a greenish blue color with the Hopkins-Cole reagent, changed to purplish red with FeCl₃ and to a vivid green-blue on dilution; Br in H₂O gives a characteristic rose-pink color, readily removed by AmOH or BuOH; attempted demethylation with HCl or H₂SO₄ gives dark brown or green amorphous products. It would appear that before the HO derivative (which, with III, is considered a biol. precursor of the Harmala alkaloids), can be obtained, a new method of synthesizing tryptophan (IV) will be necessary. 1-IV and AcH in H₂O, 12 hrs. at room temperature, give a quant. yield of 3-methyl-3,4,5,6-tetrahydro-4-carboline-5-carboxylic acid (V), m. 295-9°; oxidation gives 70% of harman. Similarly, III and AcH in H₂O, gently warmed for 10 min., give the 11-MeO derivative of V, with 1 mol. H₂O, m. 244-6°; oxidation gives 40% of harmine. Attempts to decarboxylate V have been unsuccessful, which would indicate that the tetrahydropyridine ring is formed after, rather than before decarboxylation has occurred.

IT 858786-93-3P, Hydantoin, 5-[(6-methoxy-3-indolylmethylene)-
RL: PREP (Preparation)
(preparation of)
RN 858786-93-3 CAPLUS
CN 2,4-Imidazolidinedione, 5-[(6-methoxy-1H-indol-3-yl)methylene]- (CA INDEX NAME)



=> D IBIB ABS HITSTR L30 1062

L30 ANSWER 1062 OF 1069 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1939:8714 CAPLUS

DOCUMENT NUMBER: 33:8714

ORIGINAL REFERENCE NO.: 33:1316h-i,1317a

TITLE: Synthesis of r- α -methylamino- β -3-indolylpropionic acid

AUTHOR(S): Miller, Eric J.; Robson, Wm.

SOURCE: Journal of the Chemical Society (1938) 1910-12

CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Glycine (19 g.) in 375 ml. of 2 N NaOH and 40 mols. of PhSO₂Cl (mixed with shaking), treated with 25 g. of solid NaOH and 48 ml. Me₂SO₄, give 87.5% of N-benzenesulfonylsarcosine (I). I (40 g.), refluxed with 95 ml. 50% H₂SO₄ for 4-5 hrs., gives 1-methylglycine which with 14 g. KCNO yields 72% of 1-methylhydantoin (II), m. 157-9°. Refluxing 5 g. of indole-3-aldehyde, 5 g. II and 10 ml. piperidine for 1 hr. gives a quant. yield of 5-(3'-indolal)-1-methylhydantoin (III), m. 337-8°.

Reduction of III with H₂S and concentrated NH₄OH (heating at 100-5° for 3 days and repeating the procedure twice) gives 80% of the 5-(3'-indolylmethyl) derivative, m. 211-12°, which was hydrolyzed by refluxing with Ba(OH)₂ for 20 hrs., giving 90% of α-methylamino-β-3-indolylpropionic acid, m. 245° (decomposition).

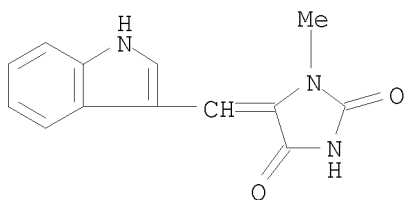
IT 91902-09-9P, Hydantoin, 5-(3-indolylmethylene)-1-methyl-

RL: PREP (Preparation)

(preparation of)

RN 91902-09-9 CAPLUS

CN Hydantoin, 5-(indol-3-ylmethylene)-1-methyl- (7CI) (CA INDEX NAME)



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	ENTRY	SESSION
FULL ESTIMATED COST	52.89	908.97
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